



A second-order accurate numerical approximation for the fractional diffusion equation

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Abstract

Fractional order diffusion equations are generalizations of classical diffusion equations, treating super-diffusive flow processes. In this paper, we examine a practical numerical method which is second-order accurate in time and in space to solve a class of initial-boundary value fractional diffusive equations with variable coefficients on a finite domain. An approach based on the classical Crank–Nicholson method combined with spatial extrapolation is used to obtain temporally and spatially second-order accurate numerical estimates. Stability, consistency, and (therefore) convergence of the method are examined. It is shown that the fractional Crank–Nicholson method based on the shifted Grünwald formula is unconditionally stable. A numerical example is presented and compared with the exact analytical solution for its order of convergence.

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1. Introduction

Consider a one-dimensional fractional diffusion equation

$$\frac{\partial u(x, t)}{\partial t} = d(x) \frac{\partial^\alpha u(x, t)}{\partial x^\alpha} + q(x, t) \quad (1)$$

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on a finite domain $x_L < x < x_R$ with $1 < \alpha \leq 2$. We assume that the diffusion coefficient (or diffusivity) $d(x) > 0$. We also assume an initial condition $u(x, t = 0) = s(x)$ for $x_L < x < x_R$ and Dirichlet boundary conditions of the form $u(x_L, t) = 0$ and $u(x_R, t) = b_R(t)$. The fractional derivative in Eq. 1 is a (left-sided) Riemann fractional derivative over the x domain. For a function $f(x)$ over the interval $L < x < R$, the Riemann fractional derivative of order α , is defined by

$$\frac{d^\alpha f(x)}{dx^\alpha} = \frac{1}{\Gamma(n - \alpha)} \frac{d^n}{dx^n} \int_L^x \frac{f(\xi)}{(x - \xi)^{\alpha+1-n}} d\xi, \quad (2)$$

where n is an integer such that $n - 1 < \alpha \leq n$. See [12,13] for details. We assume that $L \leq x_L$ and $x_R \leq R$, and since $u(x_L, t) = 0$, we can zero-extend the solution to $x < x_L$ so that the actual value of L is unimportant.

In the analysis of the numerical method that follows, we will assume that (1) has a unique and sufficiently smooth solution. Note that $\alpha = 2$ is the classical diffusion equation. The case of $1 < \alpha < 2$ models a superdiffusive flow in which a cloud of diffusing particles spreads at a faster rate than the classical diffusion model predicts [8,11], and $\alpha = 1$ corresponds to the classical advective flow. Other one-dimensional fractional diffusion equations exist that contain a right-sided or symmetric fractional derivative term, and the methods in this paper may also be useful in that context, see Remark 4.1 for a discussion.

Several different first-order accurate numerical methods to solve fractional diffusion equations have been presented before [3,4,6,7,9,10]. Many finite difference approximations for the fractional difference equations are based on some form of the Grünwald estimates, and these estimates are only first-order accurate. We are not aware of any published finite-difference methods for these differential equations which offer better than first-order accuracy. A hybrid second-order (in time and space) numerical method, which combines a fractional Crank–Nicholson method with the extrapolation of the Crank–Nicholson solution, is presented here. This method is also proven to be consistent and unconditionally stable.

2. The Crank–Nicholson method for the fractional diffusion equation

We discretize the spatial α -order fractional derivative using the Grünwald finite difference formula [12]. The standard Grünwald estimates generally yield unstable finite difference equations regardless of whether the resulting finite difference method is an explicit or an implicit system, see [9] for related discussion. Therefore, we use a right-shifted Grünwald formula to estimate the spatial α -order fractional derivative

$$\frac{\partial^\alpha u(x, t)}{\partial x^\alpha} = \frac{1}{\Gamma(-\alpha)} \lim_{N \rightarrow \infty} \frac{1}{h^\alpha} \sum_{k=0}^N \frac{\Gamma(k - \alpha)}{\Gamma(k + 1)} u(x - (k - 1)h, t), \quad (3)$$

where N is a positive integer, $h = (x - x_L)/N$ and $\Gamma(\cdot)$ is the gamma function.

For the Crank–Nicholson numerical approximation scheme, define $t_n = n\Delta t$ to be the integration time $0 \leq t_n \leq T$, and $\Delta x = h > 0$ to be the grid size in x -direction, $\Delta x = (x_R - x_L)/N_x$, with $x_i = x_L + i\Delta x$ for $i = 0, \dots, N_x$. Define $u_i^n = u(x_i, t_n)$, $d_i = d(x_i)$, and $q_i^{n+1/2} = q(x_i, t_{n+1/2})$.

Let U_i^n denote the numerical approximation to the exact solution u_i^n .

We also define the ‘normalized’ Grünwald weights by

$$g_{\alpha,k} = \frac{\Gamma(k - \alpha)}{\Gamma(-\alpha)\Gamma(k + 1)}. \quad (4)$$

For example, the first four terms of this sequence are given by $g_{\alpha,0} = 1$, $g_{\alpha,1} = -\alpha$, $g_{\alpha,2} = \alpha(\alpha - 1)/2!$, $g_{\alpha,3} = -\alpha(\alpha - 1)(\alpha - 2)/3!$

If the shifted Grünwald estimates are substituted in the superdiffusion problem (1) to get the Crank–Nicholson type numerical approximation, the resulting finite difference equations are

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} = \frac{d_i}{2} (\delta_{\alpha,x} U_i^{n+1} + \delta_{\alpha,x} U_i^n) + q_i^{n+1/2}, \tag{5}$$

where the above fractional partial differentiation operator is defined as

$$\delta_{\alpha,x} U_i^n = \frac{1}{(\Delta x)^\alpha} \sum_{k=0}^{i+1} g_{\alpha,k} U_{i-k+1}^n,$$

which is an $O(\Delta x)$ approximation to the α -order fractional derivative (see Proposition 3.1 in this paper).

Eq. (5) may be re-arranged and written as the fractional Crank–Nicholson discretization in the form

$$\left(1 - \frac{d_i \Delta t}{2} \delta_{\alpha,x}\right) U_i^{n+1} = \left(1 + \frac{d_i \Delta t}{2} \delta_{\alpha,x}\right) U_{i,j}^n + q_i^{n+1/2} \Delta t. \tag{6}$$

Note that for the classical diffusion equation, ($\alpha = 2$), the weights $g_{2,k}$ vanish for $k > 2$ and the shifted Grünwald estimate results in the classical Crank–Nicholson method for which

$$\delta_{2,x} U_i^n = \frac{U_{i+1}^n - 2U_i^n + U_{i-1}^n}{(\Delta x)^2}$$

becomes an $O((\Delta x)^2)$ approximation to the second spatial derivative. There is no analogous second-order finite difference formula in the fractional case, so we will employ (see Section 4 in this paper) a Richardson extrapolation scheme in the x -direction to obtain second-order accuracy in spatial direction.

The operator form (6) may be written in matrix form and solved to obtain the numerical solution at the time step t_{n+1}

$$(I - A)\underline{U}^{n+1} = (I + A)\underline{U}^n + \underline{Q}^{n+1/2} \Delta t, \tag{7}$$

where

$$\begin{aligned} \underline{U}^n &= [U_1^n, \dots, U_{N_x-1}^n]^T, \\ \underline{Q}^{n+1/2} \Delta t &= [q_1^{n+1/2} \Delta t, q_2^{n+1/2} \Delta t, \dots, q_{N_x-1}^{n+1/2} \Delta t + \eta_{N_x-1} (b_R^{n+1} + b_R^n)]^T \end{aligned}$$

and I is the $(N_x - 1) \times (N_x - 1)$ identity matrix. Note that the boundary conditions are absorbed in the definition of the vector \underline{Q} , with $b_R^n = b_R(t_n)$ at the right boundary.

Discretization at the interior x -gridpoints defines the matrix A entries, $A_{i,j}$ for $i = 1, \dots, N_x - 1$ and $j = 1, \dots, N_x - 1$ by

$$A_{i,j} = \begin{cases} \eta_i g_{\alpha,i-j+1} & \text{for } j \leq i - 1, \\ \eta_i g_{\alpha,1} & \text{for } j = i, \\ \eta_i g_{\alpha,0} & \text{for } j = i + 1, \\ 0 & \text{for } j > i + 1, \end{cases}$$

where

$$\eta_i = \frac{d_i \Delta t}{2(\Delta x)^\alpha}. \tag{8}$$

Note that this fractional Crank–Nicholson discretization approach will produce a method with a local truncation error that is $O((\Delta t)^2) + O(\Delta x)$. For a proof of first-order truncation error for the spatial fractional derivative term using the shifted Grünwald estimate, see Proposition 3.1 in this paper. In the classical case of $\alpha = 2$ the spatial truncation error contribution becomes $O((\Delta x)^2)$.

Remark 2.1. The coefficient matrix $(I - A)$ is a super-triangular matrix. That is, it is the sum of a super-diagonal matrix and a lower triangular matrix. The computational work in solving this system of equations is equivalent to solving two triangular systems at each time step, leading to an efficient solution algorithm which requires no pivoting due to its strict diagonal dominance (see proof of Proposition 3.3 in this paper). Note that if the fractional differential equation involves both the left-sided and the right-sided fractional derivatives, the resulting coefficient matrix will be a full matrix and no longer super-triangular.

3. Consistency and stability analysis of the fractional CN

The following proposition, regarding the Taylor expansion for the error in the shifted Grünwald finite difference formula, will be needed to establish the second-order convergence of the extrapolation method in the following section. The result is only proven for the case $L = -\infty$ in (2), but this is sufficient for our purposes. The zero Dirichlet boundary condition on the left, together with a zero-extension of the solution for $x < x_L$, implies that any value of $L \leq x_L$ gives the same solution to the fractional diffusion Eq. (1) in this case.

Proposition 3.1. *Let $1 < \alpha < 2$, $f \in C^{n+3}(\mathbb{R})$ such that all derivatives of f up to order $n + 3$ belong to $L^1(\mathbb{R})$. For any integer $p \geq 0$ define the shifted Grünwald difference operator by*

$$\Delta_{h,p}^\alpha f(x) = \sum_{j=0}^\infty (-1)^j \binom{\alpha}{j} f(x - (j - p)h). \tag{9}$$

Then if $L = -\infty$ in (2), we have for some constants a_l independent of h, f, x that

$$h^{-\alpha} \Delta_{h,p}^\alpha f(x) = \frac{d^\alpha}{dx^\alpha} f(x) + \sum_{l=1}^{n-1} \left(a_l \frac{d^{\alpha+l}}{dx^{\alpha+l}} f(x) \right) h^l + O(h^n) \tag{10}$$

uniformly in $x \in \mathbb{R}$.

Proof. The proof closely follows the result in [17] for the un-shifted Grünwald difference equations. First observe that by the Riemann–Lebesgue lemma, our assumptions on f imply that for some constant $C_1 > 0$ we have

$$|\hat{f}(k)| \leq C_1(1 + |k|)^{-n-3} \tag{11}$$

for all $k \in \mathbb{R}$, where $\mathcal{F}(f)(k) = \hat{f}(k) = \int_{\mathbb{R}} f(x) e^{ikx} dx$ denotes the Fourier-transform. Moreover, note that if $L = -\infty$ in (2), then $\mathcal{F}\left(\frac{d^\alpha}{dx^\alpha} f(x)\right)(k) = (-ik)^\alpha \hat{f}(k)$ generalizing the well-known formula for the Fourier-transform of an integer-order derivative. Observe further that for any $a \in \mathbb{R}$ we have $\mathcal{F}[f(x - a)](k) = e^{iak} \hat{f}(k)$ and that

$$(1 + z)^\alpha = \sum_{j=0}^\infty \binom{\alpha}{j} z^j$$

converges absolutely for $|z| \leq 1$. Hence $\Delta_{h,p}^\alpha f \in L^1(\mathbb{R})$ and therefore

$$\begin{aligned} \mathcal{F}\left(h^{-\alpha} \Delta_{h,p}^\alpha f\right)(k) &= h^{-\alpha} e^{-ikph} \sum_{j=0}^\infty (-1)^j \binom{\alpha}{j} e^{ijkh} \hat{f}(k) = h^{-\alpha} e^{-ikph} (1 - e^{ikh})^\alpha \hat{f}(k) \\ &= (-ik)^\alpha \left(\frac{1 - e^{ikh}}{-ikh} \right)^\alpha e^{-ikhp} \hat{f}(k) = (-ik)^\alpha \omega_{\alpha,p}(-ikh) \hat{f}(k), \end{aligned} \tag{12}$$

where $\omega_{x,p}(z) = \left(\frac{1-e^{-z}}{z}\right)^\alpha e^{pz}$. Since $\omega_{x,p}(z)$ is analytic in some neighborhood of the origin we have the power series expansion $\omega_{x,p}(z) = \sum_{l=0}^\infty a_l z^l$, which converges absolutely for all $|z| \leq R$ and some $R > 0$. Note that $a_0 = 1$ and that $a_1 = -\alpha/2 + p$. Next we show that there exists a constant $C_2 > 0$ such that

$$\left| \omega_{x,p}(-ix) - \sum_{l=0}^{n-1} a_l (-ix)^l \right| \leq C_2 |x|^n \tag{13}$$

uniformly in $x \in \mathbb{R}$: For $|x| \leq R$ we have

$$\left| \omega_{x,p}(-ix) - \sum_{l=0}^{n-1} a_l (-ix)^l \right| = \left| \sum_{l=n}^\infty a_l (-ix)^l \right| \leq |x|^n \sum_{l=n}^\infty |a_l| |x|^{l-n} \leq C_3 |x|^n,$$

where $C_3 = R^{-n} \sum_{l=0}^\infty |a_l| R^l < \infty$, while for $|x| > R$ we have

$$|\omega_{x,p}(-ix)| = \left| \left(\frac{1-e^{ix}}{-ix}\right)^\alpha e^{-ipx} \right| \leq \frac{2^\alpha}{R^\alpha} \leq C_4 |x|^n,$$

where $C_4 = 2^\alpha / R^{\alpha+n} < \infty$, and

$$\left| \sum_{l=0}^{n-1} a_l (-ix)^l \right| \leq |x|^n \sum_{l=0}^{n-1} |a_l| |x|^{l-n} \leq C_5 |x|^n,$$

where $C_5 = \sum_{l=0}^{n-1} |a_l| R^{l-n} < \infty$. Now if we set $C_2 = \max\{C_3, C_4 + C_5\}$ then it follows easily that (13) holds for all $x \in \mathbb{R}$.

In view of (12) we can write

$$\mathcal{F}\left(h^{-\alpha} \Delta_{h,p}^\alpha f\right)(k) = \sum_{l=0}^{n-1} a_l (-ik)^{\alpha+l} h^l \hat{f}(k) + \hat{\varphi}(k, h),$$

where

$$\hat{\varphi}(k, h) = (-ik)^\alpha \left(\omega_{x,p}(-ikh) - \sum_{l=0}^{n-1} a_l (-ikh)^l \right) \hat{f}(k).$$

Note that by (11) we have $(-ik)^{\alpha+l} \hat{f}(k) \in L^1(\mathbb{R})$ for $0 \leq l \leq n-1$. Moreover, in view of (11) and (13) we know that $\hat{\varphi}(k, h) \in L^1(\mathbb{R})$ with $|\hat{\varphi}(k, h)| \leq Ch^n (1 + |k|)^{\alpha-3}$ for $k \in \mathbb{R}$, with $C = C_1 C_2$. By Fourier inversion we therefore get

$$h^{-\alpha} \Delta_{h,p}^\alpha f(x) = \frac{d^\alpha}{dx^\alpha} f(x) + \sum_{l=1}^{n-1} a_l \frac{d^{\alpha+l}}{dx^{\alpha+l}} f(x) h^l + \varphi(x, h),$$

where

$$|\varphi(x, h)| = \left| C \int_{\mathbb{R}} e^{-ikx} \hat{\varphi}(k, h) dk \right| \leq C \int_{\mathbb{R}} |\hat{\varphi}(k, h)| dk \leq Ch^n$$

uniformly in $x \in \mathbb{R}$. This concludes the proof. \square

Remark 3.2. The integer parameter p is the number of gridpoints to the right of the point x_i which are used in computing the α th partial derivative at x_i . Although the theorem is stated here for the general case with any number of shifts, for the problem of interest here where $1 < \alpha < 2$, a value $p = 1$ is used. This finite difference formula generally gives the smallest local error, and it neither requires the solution values past the right boundary nor the use of different estimators as the right boundary is approached. For $p = 1$ and $\alpha = 2$, the classical centered finite difference formula is obtained.

Proposition 3.3. *The fractional Crank–Nicholson discretization, using the shifted Grünwald estimates, applied to the fractional diffusion Eq. (1) and defined by (7) is unconditionally stable for $1 < \alpha < 2$.*

Proof. We will first show that the (complex-valued) eigenvalues of the matrix A have negative real parts. Note that $g_{\alpha,1} = -\alpha$, and for $1 < \alpha < 2$ and $i \neq 1$ we have $g_{\alpha,i} > 0$. Additionally, $-g_{\alpha,1} = \alpha \geq \sum_{k=0, k \neq 1}^{k=N} g_{\alpha,i}$ for any $N > 1$. According to the Greschgorin theorem ([5] pp. 135–136), the eigenvalues of the matrix A are in the disks centered at each diagonal entry $A_{i,i} = \eta_i$, $g_{\alpha,1} = -\eta_i \alpha$, with radius

$$r_i = \sum_{j=0, j \neq i}^{N_x} |A_{i,j}| = \eta_i \sum_{j=0, j \neq i}^{i+1} g_{\alpha, i-j+1} < \eta_i \alpha.$$

These Greschgorin disks are within the left half of the complex plane. Therefore, the eigenvalues of the matrix A have negative real parts.

Next, λ is an eigenvalue of matrix A if and only if $(1 - \lambda)$ is an eigenvalue of the matrix $(I - A)$, if and only if $(1 + \lambda)/(1 - \lambda)$ is an eigenvalue of the matrix $(I - A)^{-1}(I + A)$. We observe that the first part of this statement implies that all the eigenvalues of the matrix $(I - A)$ have a magnitude larger than 1, and thus this matrix is invertible. Furthermore, since the real part of λ is negative, it is not hard to check that $|\frac{1+\lambda}{1-\lambda}| < 1$. Therefore, the spectral radius of the system matrix $(I - A)^{-1}(I + A)$ is less than one. Thus, the system of finite difference Eq. (7) is unconditionally stable. \square

Remark 3.4. The classical stability analysis of the Crank–Nicholson method for the diffusion equation relies on an eigenfunction expansion of the second derivative operator [16]. It may also be possible to develop a similar theory for the fractional diffusion equation using the fact that the Mittag–Leffler functions are the eigenfunctions of the Caputo fractional derivative [1]. However, this requires reformulating the fractional diffusion equation in terms of the Caputo derivative instead of the Riemann fractional derivative, and we have not attempted this.

4. Improving the order of convergence of the fractional Crank–Nicholson method by extrapolation

The fractional Crank–Nicholson was shown to be stable above. This method is consistent with a local truncation error which is $O((\Delta t)^2) + O(\Delta x)$. Therefore, according to Lax’s Equivalence Theorem [16], it converges at this rate. If $\alpha = 2$, then the standard spatially second-order accurate Crank–Nicholson method is obtained. To improve the low order of spatial convergence for non-integer values of $1 < \alpha < 2$, we employ an extrapolation method only at the timestep where the numerical solution is desired in the spatial direction. Proposition 3.1 shows that the error in the shifted Grünwald finite difference approximation is $C_1 \Delta x + C_2 (\Delta x)^2 + O(\Delta x)^3$ where the coefficients C_i do not depend on the grid size Δx . Hence, if the Crank–Nicholson method is applied at a grid size $h = \Delta x$ and again at a grid size $h/2$, the Richardson extrapolation method (see, e.g. [5]) can be used to obtain a solution with local truncation error $O((\Delta t)^2) + O((\Delta x)^2)$ even in the fractional case. More specifically, we apply the Crank–Nicholson method on a (coarse) grid of size $\Delta x = h$, and then on a finer grid of size $h/2$ with the same Δt . The extrapolated solution is then computed from $U_x = 2U_{x,h/2} - U_{x,h}$, where x is a grid point on the coarse mesh, and $U_{x,h}$, $U_{x,h/2}$ denote the Crank–Nicholson solutions at the grid point x using the coarse grid (grid size h) and the fine grid (grid size $h/2$), respectively. In other words, $x = x_i$ on the coarse grid, while $x = x_{2i}$ on the fine grid, so that $U_{x,h} = U_{x_i,h}$, and $U_{x,h/2} = U_{x_{2i},h/2}$.

Remark 4.1. The fractional diffusion Eq. (1) employs a left-sided fractional derivative. Other one-dimensional fractional diffusion equations (see, e.g. Schumer et al. [15]) contain an additional diffusion term, which relies

on the right-sided fractional derivative. See [13,14] for the definition of the right-sided fractional derivative. An important special case of these two-sided fractional diffusion equations uses the symmetric fractional derivative, which is just the sum of the left-hand and right-hand derivatives. See Chechkin et al. [2] for a recent application. A first-order implicit Euler finite difference method for two-sided fractional diffusion equations was developed in [10]. It should also be possible to apply the methods in this paper to these equations, in order to achieve second-order convergence in space and time, but we have not attempted this.

5. A Numerical Example

The following fractional ($\alpha = 1.8$) differential equation was considered

$$\frac{\partial u(x,t)}{\partial t} = d(x) \frac{\partial^{1.8} u(x,t)}{\partial x^{1.8}} + q(x,t)$$

on a finite domain $0 < x < 1$, with the diffusion coefficient

$$d(x) = \Gamma(2.2)x^{2.8}/6 = 0.183634x^{2.8},$$

the source/sink function

$$q(x,t) = -(1+x)e^{-t}x^3,$$

the initial condition

$$u(x,0) = x^3 \quad \text{for } 0 < x < 1$$

and the boundary conditions

$$u(0,t) = 0, \quad u(1,t) = e^{-t} \quad \text{for } t > 0.$$

Note that the exact solution to this problem is

$$u(x,t) = e^{-t}x^3,$$

which can be verified by direct fractional differentiation of the given solution and substituting in the fractional differential equation (the initial and the boundary conditions are clearly satisfied). This example problem was solved to time $t = 1.0$.

Fig. 1 shows the (unextrapolated) numerical solution obtained by applying the fractional Crank–Nicholson method (7) discussed above, with $\Delta t = 1/10$ and $\Delta x = h = 1/10$, at time $t = 1.0$. The numerical solution compares well with the exact analytic solution to the fractional partial differential equation in this test case.

To examine the rate of convergence for this method, we started with a $\Delta t = 1/10$ and $\Delta x = h = 1/10$. To obtain the extrapolated CN solution on this grid size, the problem was numerically solved on a (coarse) grid, and then on a finer grid size with the same Δt , while halving the Δx (that is, $\Delta t = 1/10$ and $\Delta x = h = 1/20$ for the starting grid size). The extrapolated solution is then computed for the points on the coarse grid from $U_{x_i} = 2U_{x_{2i},h/2} - U_{x_i,h}$.

Table 1 shows the absolute error for the numerical solutions. The third column shows the absolute value of the largest error in the numerical solution at time $t = 1.0$. The fourth column shows the ratio of the error reduction as the grid is refined. Note that the behavior of this error is (almost) linear when the Crank–Nicholson method is used and that the second-order convergence in time T is masked by the linear order of convergence in x . Column five shows the largest absolute error when the Crank–Nicholson solution is

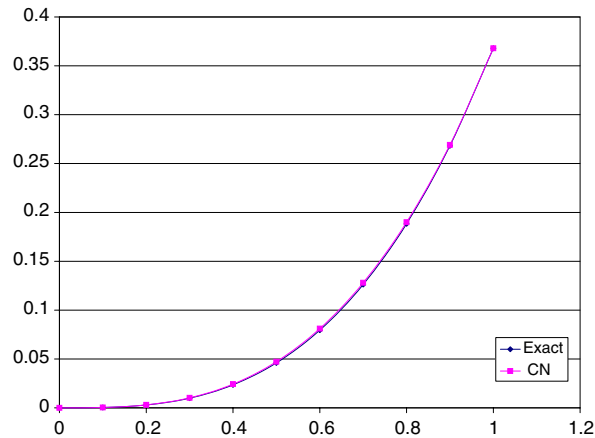


Fig. 1. Comparison of exact solution to the unextrapolated Crank–Nicholson solution at time $t = 1.0$.

Table 1

Maximum error behavior for CN and extrapolated CN and the effect of the grid size reduction at time $t = 1.0$

Δt	Δx	Max Error-CN	Error rate	Max Error-ExtCN	Error rate
1/10	1/10	1.82265×10^{-3}	–	1.77324×10^{-4}	–
1/15	1/15	1.16803×10^{-3}	$1.56 \approx 15/10$	7.85366×10^{-5}	$2.25 = (15/10)^2$
1/20	1/20	8.64485×10^{-4}	$1.35 \approx 20/15$	4.40627×10^{-5}	$1.78 = (20/15)^2$
1/25	1/25	6.84895×10^{-4}	$1.26 \approx 25/20$	2.82750×10^{-5}	$1.56 = (25/20)^2$

extrapolated. Column six shows the ratio of these extrapolated solution errors to examine the convergence, and we note that the convergence is second order $(\Delta t)^2 + (\Delta x)^2$.

The algorithm was implemented using the Intel Fortran compiler on a Dell Pentium PC. All computations were performed in single precision.

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