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# Spectral analysis of finite difference schemes for convection diffusion equation

V.K. Suman [a,*], Tapan K. Sengupta [b], C. Jyothi Durga Prasad [c], K. Surya Mohan [c], Deepanshu Sanwalia [c]

[a] CSIR-NAL, Bangalore, India
[b] High Performance Computing Lab, Aerospace engineering, IIT Kanpur, India
[c] Indian Institute of Technology Bombay, Powai, Mumbai, India

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ABSTRACT

The paper presents numerical analysis of finite difference schemes for solving the linear convection-diffusion equation using a full domain spectral analysis method illustrated in Sengupta et al. (2003) [7]. Different numerical schemes ranging from simple central and upwind difference schemes to high accuracy schemes like compact and combined compact difference schemes are analyzed for their accuracy. Optimal values of simulation parameters are proposed for the analyzed schemes with a view to obtain accurate solutions.



## 1. Introduction

Among various natural phenomena, convection, diffusion and convection-diffusion processes are the most fundamental, as they occur in a wide range of disciplines like fluid flows, climate studies, biological systems, chemical processes, energy, astrophysics etc. to name a few. The governing equations which describe them are in general non-linear and hence difficult to solve using analytical methods. Therefore, numerical techniques are employed for solution. It should be noted that the numerical solution is, in general, an approximation to the exact solution and the accuracy depends on the scheme's ability to faithfully represent the physics described by the equation. Hence, numerical analysis plays an important role, if one seeks to quantify the errors and thereby measure the accuracy of schemes. Due to the complex nature of most governing equations of convective, diffusive and convective-diffusive processes, non-linearity which introduces difficulties in analysis and non-availability of exact/reference solutions needed for comparison, one uses prototype or model equations. These model equations are the linear convection, linear diffusion and linear convection-diffusion equations, to name only a few.

Traditionally finite difference based numerical schemes have been analyzed either using von Neumann analysis [1,2] or GKS stability theory [3] or time-stability analysis [4,5]. These approaches have limitations with the most notable one being their inability to analyze in the spectral space by full domain analysis with actual time discretization method. On the other hand, a full domain spectral analysis with appropriate error metrics [6] reveals more information about stability/instability, dispersion and dissipation errors for all length and time scales. This information is extremely critical in evaluating/ designing dispersion relation preserving (DRP) schemes for direct numerical simulation (DNS)/ large eddy simulation (LES). In [7], a spectral analysis method is adopted following the approach of Vichnevetsky and Bowles [8] and different numerical schemes have been analyzed with one-dimensional linear convection equation serving as a model equation. The analysis also demonstrates an interesting property for the same model convection equation that signal and error have different dynamics [9] for any discretization scheme. In [10] error dynamics of a general finite difference based scheme for linear diffusion equation is derived and errors are quantified for some popular schemes. It is remarkable to note that the phase speed in convection equation and the coefficient of diffusion in the heat equation, do not remain constant numerically. In the present research, we will generalize these observations for convection-diffusion equation. Recently, this global spectral analysis (GSA) has been used in developing and an-

* Corresponding author.
*E-mail addresses:* vksuman@nal.res.in, sumanvajjala@gmail.com (V.K. Suman), tksen@iitk.ac.in (T.K. Sengupta).

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alyzing a positivity preserving discrete Galerkin method in [11] for convection-diffusion-reaction equation in Galerkin and least square framework.

We briefly state the reason of the present investigation on finite difference method, over other discretization techniques like finite volume and finite element methods. The focus here is to quantify error sources in solving this model convection-diffusion equation as accurately as possible. There have been earlier efforts where one-dimensional convection and Euler equations have been solved using high accuracy compact schemes for finite volume and finite difference method in [12]. It was noted specifically for the Riemann problem that the same compact scheme was superior with the finite difference method. Similar spectral analysis was reported in [13] for Galerkin finite element method, with respect to $q$-waves for different numerical methods in solving one-dimensional convection equation. While it was noted that finite element methods have good dispersion error properties, excessive diffusion causes these methods to be relatively less accurate as compared to finite difference methods.

In this paper we chose the linear 1D convection-diffusion equation as it is a closer linearized model of the governing Navier–Stokes equations of fluid dynamics. The numerical analysis of the finite difference schemes for this equation is conducted in [14–17]. However, as per our knowledge, a spectral analysis has not been performed with the appropriate metrics. It would therefore be beneficial and appropriate to analyze this equation in the spectral framework due to the advantages mentioned previously. This is the main motivation for the present work. We choose different spatial discretization schemes like explicit central, upwind, compact [7] and combined compact difference schemes [18,19], in conjunction with two different time discretization schemes- Euler and fourth order Runge–Kutta ($RK_4$) schemes, for the numerical analysis. The stability/instability regions are identified and simulation parameters for achieving good accuracy are presented. The results of the numerical analysis will have a beneficial influence on CFD and various other fields involving simulation of convection-diffusion processes.

The paper is presented in the following manner. In the next section, the global spectral analysis is illustrated for the linear 1D convection-diffusion equation and an exact spectral transfer function is derived for the equation. In Section 3, analysis of numerical schemes is presented where explicit central, upwind, compact and combined compact schemes are used for the spatial discretization and Euler, $RK_4$ schemes are adopted for the temporal discretization. In Section 4, the numerical solution of the linear convection-diffusion equation is compared to the exact solution for various simulation parameters and the results are corroborated with the findings of global spectral analyses. The paper ends with Section 5 with conclusion.

## 2. Spectral analysis of linear 1D convection-diffusion equation

We consider the linear convection-diffusion equation

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = \alpha\frac{\partial^2 u}{\partial x^2} \tag{1}$$

where $c$ and $\alpha$ are constants denoting the convection speed and coefficient of diffusion respectively. The first step in performing a global spectral analysis is to represent the unknown, $u(x, t)$, in the hybrid spectral plane [6,7], which is given by,

$$u(x,t) = \int \hat{U}(k,t)e^{ikx}dk \tag{2}$$

where $\hat{U}$ is the Fourier amplitude and $k$ is the wavenumber. Substituting this in the convection-diffusion equation we obtain the transformed equation in the spectral space given by,

$$\frac{d\hat{U}}{dt} + ick\hat{U} = -\alpha k^2\hat{U} \tag{3}$$

The above equation is solved for a general initial condition $u(x,0) = f(x) = \int \hat{F}(k)e^{ikx}dk$ to obtain the exact solution

$$\hat{U}(k,t) = \hat{F}(k)\, e^{-\alpha k^2 t}\, e^{-ikct} \tag{4}$$

To obtain the dispersion relation, we represent the unknown by the bi-dimensional Fourier–Laplace transform, i.e., $u(x,t) = \iint \hat{U}(k,\omega)e^{i(kx-\omega t)}dkd\omega$ which gives the following dispersion relation

$$\omega = ck - i\alpha k^2 \tag{5}$$

The dispersion relation is an important property for wave propagation problems and it describes the phase and group velocities for signal propagation. Hence, any numerical scheme employed to solve such problems must satisfy the physical dispersion relation for the purpose of accuracy [6,9]. Such numerical schemes are said to be DRP schemes [6]. A very concise and clear explanation of the correct dispersion relation in the context of multiple time level scheme is given in [20] for the convection equation. The same approach is followed here for the convection-diffusion equation.

From the above dispersion relation one can obtain the complex phase speed as

$$c_{phys} = \frac{\omega}{k} = c - i\alpha k \tag{6}$$

The physical group velocity as per definition is then

$$V_{g,phys} = \frac{\partial\omega}{\partial k} = c - 2i\alpha k \tag{7}$$

Therefore, $\alpha = \frac{i}{2k}(V_{g,phys} - c)$. Further expanding the real and complex parts of the complex quantities we obtain

$$\alpha = \frac{i}{2k}\left[(V_{g,phys})_{real} - c)\right] - \frac{(V_{g,phys})_{imag}}{2k} \tag{8}$$

Since $\alpha$ is real, $(V_{g,phys})_{real} = c$ is the condition for a physically diffusive system and as the right hand side of Eq. (1) is diffusive and not anti-diffusive, therefore one must have $\frac{(V_{g,phys})_{imag}}{2k} < 0$.

The physical amplification factor $G_{phys}$ can be obtained from Eq. (4) and is given by

$$G_{phys} = \frac{\hat{U}(k,t+\Delta t)}{\hat{U}(k,t)} = e^{-\alpha k^2\Delta t}\, e^{-ikc\Delta t} = e^{-i\omega\Delta t} = e^{-Pe\,(kh)^2}\, e^{-iN_c(kh)} \tag{9}$$

Note that we have purposely introduced $N_c(=\frac{c\Delta t}{h})$, which is the CFL number and $Pe(=\frac{\alpha\Delta t}{h^2})$, is the Peclet number in the above, as these are the non-dimensional parameters for this equation. The variable $h$ here is the grid spacing. The absolute part of $G$ is the amplification factor. A portrait of physical amplification factor for three values of Peclet numbers viz., $Pe = 0.05,\ 0.25$ and $0.5$ is shown in Fig. 1. We can see that as the Peclet number increases, the rate of diffusion also increases due to Eq. (9). We have not shown contours for the physical phase speed as it is exactly equal to $c$ for every wavenumber $k$.

Similarly, every numerical scheme has a corresponding amplification factor $G_{num}$, which indirectly defines a numerical dispersion relation governing the evolution of the solution. It is, therefore, clear that for a numerical scheme to faithfully reproduce the physics of the governing equations, $G_{num}$ must be very close to $G_{phys}$. In the case of the 1D linear convection-diffusion equation, the numerical dispersion relation is directly obtained by drawing analogy from Sengupta et al. [9] and Sengupta and Bhole [10] for pure convection and pure diffusion equations as,

$$\omega_{num} = kc_{num} - i\alpha_{num}k^2 \tag{10}$$