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Error dynamics of diffusion equation: Effects of numerical diffusion and dispersive diffusion

Tapan K. Sengupta *, Ashish Bhole

Department of Aerospace Engineering, Indian Institute of Technology Kanpur, Kanpur 208016, India

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ABSTRACT

An error propagation equation has been obtained for the numerical solution of an initial-boundary value problem governed by linear diffusion equation. The error propagation equation is analyzed to identify different types of errors as those due to sub- or super-diffusion and dispersive diffusion errors. Quantification of errors has also been used for numerical analysis of some central difference methods to solve this equation.

1. Introduction

As an example of hyperbolic partial difference equations (PDEs), the linear convection equation is often used as a model in numerical analysis [1–4]. The analysis in [4], established the interesting property of numerical solution, for which the signal and error do not obey same dynamics. Similarly, the linear diffusion (or heat) equation is used here as a model to analyze diffusion process given by parabolic PDEs [5–8]. Error in numerical solutions of PDEs arise due to discretization (numerical method dependent) and rounding off real numbers (hardware dependent). To minimize errors due to discretization, the knowledge of sources, behavior and quantification of these errors are necessary. Here, errors due to discrete approximations of a linear parabolic PDE is studied and correct error propagation dynamical equation is obtained, as it was performed in [4] for hyperbolic equation.

Traditional analysis attributed to von Neumann for linear problems [9,10], assumes error to follow the same dynamics as given by governing difference equation for the signal. However it is shown in [4] that the governing error propagation equation is different from the governing dynamics of 1D convection equation for the signal. The most significant result of [4] is to identify the correct error propagation equation as a forced dynamics problem with product terms in wavenumber (k)-plane as sources. This equation accounts for dissipation, dispersion and phase errors. For linear PDEs, notable references for stability analysis are [1,6–8,11] and for error analysis are as in [2,4,12–14]. The motivation behind the present work is to introduce correct error dynamics for parabolic PDEs using diffusion equation to identify set of parameters for numerical analysis. In [2], authors have studied amplitude and phase errors for error analysis of 1D convection equation. In [4,12–14], a set of parameters have been identified for error analysis of 1D convection equation which accounts for neutral stability, phase and dispersion errors. Here, we have obtained governing error dynamics for 1D linear diffusion equation and shown

* Corresponding author. Tel.: +91 512 2597945.
E-mail address: tksen@iitk.ac.in (T.K. Sengupta).

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once again that the error propagation dynamics is not given by the original PDE. As an outcome of this, the correct error propagation equation is noted to depend upon diffusion error and dispersive diffusion effects.

Many physical phenomena such as diffusion and heat conduction in isotropic medium, fluid flow through porous media, boundary layer flow over a flat plate, persistence of solar prominence, and the growth of wake behind submerged objects have been modeled by parabolic PDEs [5]. Therefore, numerical analysis performed here is directly applicable for computations of parabolic PDEs.

2. Error dynamics for linear 1D diffusion equation

Analysis of space–time discretization of 1D diffusion equation with constant coefficient of diffusivity (ν) is used as a model for parabolic PDE

$$\frac{\partial u}{\partial t} - \nu \frac{\partial^2 u}{\partial x^2} = 0, \quad \nu > 0 \tag{1}$$

with the initial condition given by, $u(x_j, 0) = f(x)$ for $-\infty < x < \infty$. Using hybrid spectral representation, one writes $u(x,t) = \int U(k,t) e^{ikx}\, dk$ and transforms Eq. (1) as

$$U_t + \nu k^2 U = 0$$

This is a first order equation in U and solved for the given initial condition $f(x) = \int A_0(k) e^{ikx}\, dk$ to obtain the solution in spectral plane as

$$U = A_0 e^{-\nu k^2 t} \tag{2}$$

The exact solution of Eq. (1) for the given initial condition $f(x)$ is given in physical plane as

$$u(x,t) = \int_{-\infty}^{\infty} f(y) e^{\frac{(x-y)^2}{4\nu t}}\, dy \tag{3}$$

If we represent $u(x,t)$ by its Fourier–Laplace transform as, $u(x,t) = \iint \hat{U}(k,\omega) e^{i(kx-\omega t)}\, dk\, d\omega$, then the dispersion relation for Eq. (1) is

$$\omega = -i\nu k^2 \tag{4}$$

The unknown can be represented by hybrid form at the jth node of a uniformly spaced discrete grid of spacing h as, $u(x_j,t) = \int U(k,t) e^{ikx_j}\, dk$, for which the exact second derivative at the same node is given by, $[u''(x_j,t)]_{exact} = -\int k^2 U(k,t) e^{ikx_j}\, dk$, which numerically can be shown as equivalent to [1,12]

$$\left[u''(x_j,t)\right]_{numerical} = -\int k_{eq}^{(2)} U(k,t) e^{ikx_j}\, dk \tag{5}$$

When Eq. (1) is approximated by discrete methods, spatial derivative u_j'' can also be denoted as $\{u''\} = \frac{1}{h^2}[C]\{u\}$, with $[C]$ obtained for finite-domain non-periodic problems and the dimension N of $[C]$ is equal to the number of nodes. Thus, the derivative at jth node is $u_j'' = \frac{1}{h^2}\sum_{l=1}^{N} C_{jl} u_l$, where $u_l = u(x_l, t)$ is evaluated at the lth node. Therefore, one alternatively writes the numerical derivative as

$$u_j'' = \int \frac{1}{h^2} \sum_{l=1}^{N} C_{jl} U(k,t) e^{ik(x_l - x_j)} e^{ikx_j}\, dk \tag{6}$$

Comparing Eq. (5) with (6), it can be noted that

$$\left[k_{eq}^{(2)}\right]_j = -\frac{1}{h^2} \sum_{l=1}^{N} C_{jl} e^{ik(x_l - x_j)}$$

In general, $[k_{eq}^{(2)}]$ is a complex number, with real part indicating diffusion and the imaginary part is the undesirable numerical dispersion. These quantities depend on the entries of the matrix $[C]$. Other numerical properties are obtained in spectral plane for Eq. (1) as

$$\int \left[\frac{dU}{dt} - \frac{\nu}{h^2} \sum_{l=1}^{N} U C_{jl} e^{ikx(x_l - x_j)}\right] e^{ikx_j}\, dk = 0 \tag{7}$$