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Project Proposal:

Mixed Equations:
Strang Splitting Method vs. IMEX Schemes,
A Comparison

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1 Introduction

In this project we will analyze different schemes to numerically solve mixed equations. Specifically, we will numerically solve the advection-diffusion equation in one spatial dimension, by implementing the so-called Strang-Splitting Method, for which we will use the Lax-Wendroff scheme to deal with the advection operator, and the Crank-Nicolson scheme to deal with the diffusion operator. Moreover, we will implement an Implicit-Explicit scheme, where the second-order Adams-Bashforth method will be the explicit solver, while the Crank-Nicolson scheme will be the implicit one. Our focus will be on drawing a comparison between the methods in terms of accuracy, stability and running time, in order to provide insights on how to design schemes to solve partial differential equations characterized by a mixture of physical behaviors.

1.1 Background and Motivation

In the physical world, many processes as diffusion, reaction or advection, happen simultaneously, and cannot be fully described by models that only capture one aspect of their dynamics [1]. Therefore, while we traditionally classify Partial Differential Equations (PDEs) in hyperbolic (advection equation), parabolic (heat equation) and elliptic (Laplace's Equation), in order to study phenomena characterized by different physical processes, one often has to rely on a mixture of those types of equations. In this work, we analyze

$$(u(x,t))_t + a(x)(u(x,t))_x = (\kappa(x)(u(x,t))_x)_x, \tag{1}$$

which is called the advection-diffusion equation. Eq. (1) describes the time evolution of a quantity $u(x,t)$, say the concentration of a given chemical species for instance, as it is carried (advected) by a flow, as it also diffuses. Here $a(x)$ is the speed at which $u(x,t)$ travels, while $\kappa(x,t)$ is the diffusion coefficient. For simplicity, in our work we will let $a(x) = a$ and $\kappa(x) = \kappa$, so that we can re-write Eq. (1) as

$$u_t + au_x = \kappa u_{xx}, \tag{2}$$

where we dropped the independent variables for ease of notation. In solving Eq. (2) we may want to consider different treatments of the advection operator ∂_x and the diffusion operator ∂_{xx}, and this is where Splitting methods [2] and Implicit-Explicit (IMEX) schemes [1] will prove themselves to be valuable.

2 Numerical Methods: Outline

In solving Eq. (2) we want to handle the stiffness of the diffusion operator ∂_{xx} and the advection operator ∂_x separately. To this end, we implement a fractional step method known as Strang-Splitting, and an IMEX scheme in which we use the Crank-Nicolson method (implicit) to treat diffusion and the second-order Adams-Bashforth method (explicit) to deal with the advection operator.

2.1 Strang-Splitting

Rewriting Eq. (2) in operator notation yields

$$u_t = \mathcal{A}u + \mathcal{B}u, \tag{3}$$

where $\mathcal{A} = -a\partial_x$ and $\mathcal{B} = \kappa\partial_{xx}$. The key idea behind operator splitting is to decouple the different physical effects by breaking the equation into pieces, and alternate between advancing simpler equations in time. For instance, on very small time steps, diffusion will likely act independently of advection, and vice versa [3], therefore we can write a split method of the form

$$\begin{aligned} U^\star &= \mathcal{N}_\mathcal{A}(U^n, k) \\ U^{n+1} &= \mathcal{N}_\mathcal{B}(U^\star, k), \end{aligned} \tag{4}$$

where $\mathcal{N}_\mathcal{A}$ and $\mathcal{N}_\mathcal{B}$ are the numerical methods that solve $u_t = \mathcal{A}[u]$ and $u_t = \mathcal{B}[u]$ at each time step k, respectively. Thus, for Eq. (2), one can resolve the advection part using an explicit scheme like Lax-Wendroff at time t_n to obtain $U^\star$ from Eq. (4). Then, one can use an implicit method, like Crank-Nicolson to treat the diffusion term and obtain U^{n+1}. A comprehensive discussion of fractional methods of the form as in Eq. (4) can be found in Refs.[1][3]. While these schemes are both useful in practice and serve as a good pedagogical tool for the discussion of splitting methods, in this project we will focus on an inherently more accurate splitting technique, introduced in 1968 by Gilbert Strang in [4] and called Strang-Splitting. In this scheme, we perform the fractional step

$$\begin{aligned} U^{\star} &= \mathcal{N}_{\mathcal{A}}(U^n, k/2) \\ U^{\star\star} &= \mathcal{N}_{\mathcal{B}}(U^{\star}, k) \\ U^{n+1} &= \mathcal{N}_{\mathcal{A}}(U^{\star\star}, k/2). \end{aligned} \tag{5}$$

This essentially cuts the time-step in half and drops the error down by an order of magnitude, when compared to splitting methods like Eq. (4); see Refs.[1],[3]. Therefore, to solve Eq. (2) using this method, one solves the advection for step-leght of $k/2$ to obtain $U^{\star}$, then use this solution to treat the diffusion term over a full time step k to obtain $U^{\star\star}$, and finally use this solution to solve the advection equation over half a time step once again.
In this work we will implement the Lax-Wendroff scheme to handle advection, and the Crank-Nicolson scheme to treat diffusion.

2.2 IMEX schemes

IMEX (IMplicit-EXplicit) schemes allow for the simultaneous handling of the stiffness from the diffusion operator and the non-stiff advection operator. An implicit method is used on the stiff part, and a cheaper explicit method is used on the non-stiff part. Typically schemes of the same order are used [5].

We use IMEX schemes to solve equations of the form

$$u_t = f(u) + \kappa g(u) \tag{6}$$

where $f(u)$ is the non-stiff operator and $g(u)$ is the stiff one. The general form of a linear s-step IMEX scheme is

$$\frac{1}{k}u^{n+1} + \frac{1}{k}\sum_{j=0}^{s-1} a_j u^{n-j} = \sum_{j=0}^{s-1} b_j f(u^{n-j}) + \kappa \sum_{j=-1}^{s-1} c_j g(u^{n-j}) \tag{7}$$

where k is our timestep [6].

The following Crank-Nicolson/Adams-Bashforth (CNAB) scheme is one such IMEX method which we intend to implement. Crank Nicolson is a second-order scheme, so to match that we use the second-order Adams-Bashforth scheme, commonly called AB2.

We solve the Eq. (2) on a spacial grid $x_j = jh$ for $j = 0, 1, 2, ..., m+1$, $h = 1/(m + 1)$ and time steps $t_n = nk$ for $n = 0, 1, 2, ..., N$ and $k = 1/N$. U_j^n approximates the true solution $u(x_j, t_n)$.

Let

$$\begin{aligned} \mathcal{A}[U^n] &= \frac{\kappa}{h^2}\left(U_{j-1}^n - 2U^n + U_{j+1}^n\right) \\ \mathcal{B}[U^n] &= -\frac{a}{2h}\left(U_{j+1}^n - U_{j-1}^n\right). \end{aligned} \tag{8}$$

The expression for the second order Crank-Nicolson/Adams-Bashforth IMEX scheme then is

$$U_j^{n+1} = U_j^n + \frac{k}{2}\left(3\mathcal{B}U^n - \mathcal{B}U^{n-1}\right) + \frac{k}{2}\left(\mathcal{A}U^{n+1} + \mathcal{A}U^n\right). \tag{9}$$

Both the Strang-splitting scheme (5) and the IMEX scheme (9) are constructed using second-order methods which will make our analysis and comparison meaningful.

References

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