A Godunov-Ryabenkii Instability for a Quickest Scheme

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Abstract. We consider a finite difference scheme, called Quickest, introduced by Leonard in 1979, for the convection-diffusion equation. Quickest uses an explicit, Leith-type differencing and third-order upwinding on the convective derivatives yielding a four-point scheme. For that reason the method requires careful treatment on the inflow boundary considering the fact that we need to introduce numerical boundary conditions and that they could lead us to instability phenomena. The stability region is found with the help of one of the most powerful methods for local analysis of the influence of boundary conditions – the Godunov-Ryabenkii theory.

1 Introduction

Quickest is a finite difference scheme due to Leonard [8] that deduces this scheme using control volume arguments. Davis and Moore [2] have shown that Quickest can also be derived by considering the Δt^3 in the Taylor expansion of the time derivative and make some subsequent approximations. Morton and Sobey [10] using the exact solution of the convection diffusion equation, derived Quickest based on a cubic local approximation. Quickest scheme uses an explicit, Leith-type differencing and third-order upwinding on the convective derivatives yielding a four-point scheme. In the limit $D \to 0$ is third order accurate in time. The use of third-order upwind differencing for convection greatly reduces the numerical diffusion associated with first-order upwinding [1]. Some of the literature about Quickest used in a flow simulation can be found in [1,2,6,8,9]. The major difficulties associated with the use of Quickest scheme in multidimensions are in the application of boundary conditions, being the major reason to study the influence of a numerical boundary condition on the stability of the numerical scheme.

Fourier analysis is the standard method for analysing the stability of discretisations of an initial value on a regular structured grid. This model problem has Fourier eigenmodes whose stability needs to be analysed. If they are stable at all points in the grid, and the discretisation of the boundary conditions is also stable then for most applications the overall discretisation is stable, in the sense of Lax [12].

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The influence of the boundaries can be analysed using the Godunov-Ryabenkii theory. The Godunov-Ryabenkii theory was introduced by Godunov and Ryabenkii [3] and developed by Kreiss [7], Osher [11] and Gustafsson *et al* [4] (now also called GKS theory). In this paper we find the stability region for the Quickest scheme subject to a numerical boundary condition by applying the Godunov-Ryabenkii theory.

Consider the one-dimensional problem of convection with velocity V in the x-direction and diffusion with coefficient D:

$$\frac{\partial u}{\partial t} + V\frac{\partial u}{\partial x} = D\frac{\partial^2 u}{\partial x^2} \quad 0 \leq x < \infty, \quad t \geq 0 \tag{1}$$

$$u(x,0) = f(x) \tag{2}$$

$$u(0,t) = 0 \tag{3}$$

$$||u(\cdot,t)|| < \infty \tag{4}$$

If we choose a uniform space step Δx and time step Δt, there are two dimensionless quantities very important in the properties of the scheme:

$$\mu = \frac{D\Delta t}{(\Delta x)^2}, \qquad \nu = \frac{V\Delta t}{\Delta x}$$

ν is called the Courant (or CFL) number.

Before we describe the Quickest scheme and its numerical boundary condition, we give in the next section, a brief overview of the Godunov-Ryabenkii theory.

2 Godunov-Ryabenkii Stability Analysis

Two essential aspects of normal mode analysis for the investigation of the influence of boundary conditions on the stability of a scheme are that the initial value problem needs to be stable for the Cauchy problem which is best analysed with the von Neumann method (this means the interior scheme needs to be stable) and that its stability could be destroyed by the boundary conditions, but the converse its not possible.

In this section we give a brief description of the Godunov-Ryabenkii theory. For more detailed information about the theory we suggest [12,13,14] and specially [4]. A particular note is to be made of the work [15,16], establishing a relation between the GKS theory and group velocity.

We can approximate the problem (1)– (4) by the difference scheme

$$QU_j^n = U_j^{n+1}, \qquad j = r, r+1, \ldots \tag{5}$$

$$Q = \sum_{j=-r}^{p} a_j E^j, \quad EU_j^n = U_{j+1}^n. \tag{6}$$

where a_j are scalars.

Two important assumptions are made:

a) The scalars a_{-r} and a_p are non-singular;

b) The finite difference scheme (5) is von Neumann stable.

As Q uses r points to the left, the basic approximation can not be used at $x_0, x_1, x_2, \ldots, x_{r-1}$, so there we will have to apply boundary conditions. These can be the conditions that are given for the original problem (in our particular case is associated only with the point x_0), but they can also be difference schemes, which will then be called numerical boundary conditions. The choice of numerical boundary conditions is crucial for the stability.

Let us assume that the boundary conditions can be written as

$$U_\beta^{n+1} = \sum_{j=1}^{q} l_{\beta j} U_j^n \quad \beta = 0, 1, \ldots, r-1 \tag{7}$$

where $l_{\beta j}$ are scalars.

The eigenvalue problem associated with our approximation is:

$$z\phi_j = Q\phi_j \quad j = r, r+1, \ldots \tag{8}$$

$$z\phi_\beta = \sum_{j=1}^{q} l_{\beta j}\phi_j \quad \beta = 0, 1, \ldots, r-1 \tag{9}$$

$$||\phi||_h < \infty \tag{10}$$

Lemma 1 Godunov-Ryabenkii Condition The approximation is unstable if the eigenvalue problem (8) – (10) has an eigenvalue z with $|z| > 1$.

Consider the characteristic equation of the interior scheme

$$z - \sum_{j=-r}^{p} a_j k^j = 0. \tag{11}$$

Lemma 2 For z such that $|z| > 1$, there is no solution of equation (11) with $|k| = 1$ and there are exactly r solutions, counted according to their multiplicity, with $|k| < 1$.

A general solution of (8) – (10) is of the form

$$\phi_j = \sum_{|k_a|<1} P_a(j) k_a^j, \quad k_a = k_a(z), \quad |z| > 1 \tag{12}$$

where k_a are solutions of the characteristic equation (11). This solution depends on r free parameters $\sigma = (\sigma_1, \ldots, \sigma_r)$. $P_a(j)$ is a polynomial in j. Its order is at most $m_a - 1$ where m_a is the multiplicity of k_a.

Note that if the solutions are simple, this implies that the solution has the form

$$\phi_j = \sum_{|k_i|<1} \sigma_i k_i^j. \tag{13}$$

This form of the solution is the one that usually arises in practice.

Substituting (12) into the boundary conditions (7) yields a system of equations

$$C(z)\sigma = 0,$$

$\sigma = (\sigma_1, \ldots, \sigma_r)$ and we can rephrase Lemma 2 in the following form:

Lemma 3 The approximation is unstable if

$$\text{Det } C(z) = 0 \quad \text{for some } z \in \mathbb{C} \text{ with } \quad |z| > 1.$$

Summarising, this theory is a generalisation of the von Neumann stability analysis taking into account the influence of boundary conditions. It states that the interior scheme needs to be von Neumann stable and when considered in the half-plane $x \geq 0$, a mode k^j with $|k| > 1$ will lead to an unbounded solution in space, that is, k^j will increase without bound when j goes to infinity. Therefore $|k|$ should be lower than one, and the Godunov-Ryabenkii stability condition states that all the modes with $|k| \leq 1$, generated by the boundary conditions, should correspond to $|z| < 1$.

3 Instability of a Quickest Scheme

Consider the interior difference scheme Quickest:

$$U_j^{n+1} = [1 - \nu\Delta_0 + (\frac{1}{2}\nu^2 + \mu)\delta^2 + \nu(\frac{1}{6} - \frac{\nu^2}{6} - \mu)\delta^2\Delta_-]U_j^n, \tag{14}$$

where we use the central, backward and second difference operators: $\Delta_0 U_j := (U_{j+1} - U_{j-1})/2$, $\Delta_- U_j := U_j - U_{j-1}$ and $\delta^2 U_j := U_{j+1} - 2U_j + U_{j-1}$.

We will consider two boundary conditions: the Dirichlet boundary condition associated with the original problem, $U_0^n = 0$ and the numerical boundary condition that we need at the first point of the mesh,

$$U_1^{n+1} = [1 - \nu\Delta_0 + (\frac{1}{2}\nu^2 + \mu)\delta^2 + \nu(\frac{1}{6} - \frac{\nu^2}{6} - \mu)\delta^2\Delta_+]U_1^n, \tag{15}$$

where Δ_+ is the forward operator defined by $\Delta_+ U_j := U_{j+1} - U_j$. This numerical boundary condition is deduced by a similar method used in [10] to obtain the Quickest scheme, using a local cubic interpolation of the points U_{j-2}^n, U_{j-1}^n, U_j^n, U_{j+1}^n. On the first point we can not use this interpolation since we do not have the point U_{-1}. We do instead an interpolation of the points U_0^n, U_1^n, U_2^n, U_3^n and it gives the difference scheme (15). The use of this downwind third difference at $x = \Delta x$ does not affect accuracy because it stills based on a cubic local approximation near $x = \Delta x$ as the interior scheme. However, as we shall show, it does have penalties in terms of stability.

Let us consider the corresponding eigenvalue problem:

$$
\begin{aligned}
z\phi_j &= [1 - \nu\Delta_0 + (\frac{1}{2}\nu^2 + \mu)\delta^2 + \nu(\frac{1}{6} - \frac{\nu^2}{6} - \mu)\delta^2\Delta_-]\phi_j, \quad j \geq 2 \\
\phi_0 &= 0 \\
z\phi_1 &= [1 - \nu\Delta_0 + (\frac{1}{2}\nu^2 + \mu)\delta^2 + \nu(\frac{1}{6} - \frac{\nu^2}{6} - \mu)\delta^2\Delta_+]\phi_1. \qquad (16)
\end{aligned}
$$

The Godunov-Ryabenkii condition tell us that the system (16) has an eigenvalue z with $|z| > 1$, then the approximation (14) – (15) is not stable. By Lemma 2 we have for this approximation that the characteristic equation for the interior scheme (14) has not $k = e^{i\xi}$, ξ real for $|z| > 1$ and there are exactly two solutions $k_i,\ i = 1, 2$ with $|k_i| < 1$ for $|z| > 1$.

Consider the characteristic equation for the interior scheme (14)

$$
k^3(-c_1 + c_2 + c_3) + k^2(-z + 1 - 2c_2 - 3c_3) + k(c_1 + c_2 + 3c_3) - c_3 = 0. \quad (17)
$$

where $\quad c_1 = \nu/2, \quad c_2 = \nu^2/2 + \mu \quad$ and $\quad c_3 = \nu(1 - \nu^2 - 6\mu)/6.$

Assuming that the two solutions of the characteristic equation are distinct, any solution of (16) has the form

$$
\phi_j = \sigma_1 k_1^j(z) + \sigma_2 k_2^j(z).
$$

We want to find the solutions $k_i, i = 1, 2$ of (17), such that $|k_i(z)| < 1, i = 1, 2$ and the linear and homogeneous system

$$
\begin{aligned}
\sigma_1 + \sigma_2 &= 0 \\
\sigma_1 g(k_1, z, \mu, \nu) + \sigma_2 g(k_2, z, \mu, \nu) &= 0 \qquad (18)
\end{aligned}
$$

has a solution z with $|z| > 1$. The function $g(k, z, \mu, \nu)$ is the polynomial:

$$
g(k, z, \mu, \nu) = k^3 c_3 + k^2(-c_1 + c_2 - 3c_3) + k(1 - 2c_2 + 3c_3 - z).
$$

Since the first equation gives $\sigma_1 = -\sigma_2$, the linear homogeneous system (18) has a non-trivial solution if

$$
g(k_1, z, \mu, \nu) - g(k_2, z, \mu, \nu) = 0.
$$

Consider $k_1(z)$ and $k_2(z)$ defined as:

$$
k_1(z) = \frac{r_1}{2} + \frac{\sqrt{-3r_1^2 + 4r_2}}{2} \qquad k_2(z) = \frac{r_1}{2} - \frac{\sqrt{-3r_1^2 + 4r_2}}{2}
$$

where r_1 and r_2 are:

$$r_1(z,\mu,\nu) = \frac{(1-z)(-c_1+c_2+c_3) - 4c_1c_3 + 2c_2(c_1-c_2)}{(1-z)c_3 - 2c_1c_3 - (c_1-c_2)^2} \tag{19}$$

$$r_2(z,\mu,\nu) = \frac{(1-z)(z-1+4c_2) - (c_1^2+6c_1c_3+3c_2^2)}{(1-z)c_3 - 2c_1c_3 - (c_1-c_2)^2} \tag{20}$$

Let $f(k,z,\mu,\nu)$ denote the characteristic polynomial for the interior scheme (see (17)). After some algebraic manipulations we can prove that for $c_3 \neq 0$, $k_1(z)$ and $k_2(z)$ are solutions of

$$f(k_1,z,\mu,\nu) - f(k_2,z,\mu,\nu) = 0 \tag{21}$$

$$g(k_1,z,\mu,\nu) - g(k_2,z,\mu,\nu) = 0. \tag{22}$$

If additionally to (21) $k_1(z)$ and $k_2(z)$ verify $f(k_1,z,\mu,\nu)+f(k_2,z,\mu,\nu)=0$ then $k_1(z)$ and $k_2(z)$ are solutions of f. In that way we have two solutions of f that verify (22). Note that the characteristic polynomial f is a third order polynomial, which means we expect three roots, although we only find the analytical solution of two of them. Let $C(z,\mu,\nu) = f(k_1,z,\mu,\nu) + f(k_2,z,\mu,\nu)$. For each (μ,ν) we want to find $z_{\mu\nu}$ such that $C(z_{\mu\nu},\mu,\nu)=0$. The requirement for instability is $|z_{\mu\nu}|>1$. Experimentally we observe that the solution $z(\mu,\nu)$ lies inside $|z|=1$ for certain values of μ and ν and then crosses it at $z=-1$. We can say $z=-1$ is the value of transition from stable to unstable.

The function $C(z,\mu,\nu)$ as the form

$$\begin{aligned}C(z,\mu,\nu) = {} & r_1(z,\mu,\nu)(3r_2(z,\mu,\nu) - 2r_1^2(z,\mu,\nu))(-c_1+c_2+c_3)\\ & (2r_2(z,\mu,\nu) - r_1^2(z,\mu,\nu))(-z+1-2c_2-3c_3)\\ & + r_1(z,\mu,\nu)(c_1+c_2+3c_3) - 2c_3.\end{aligned}$$

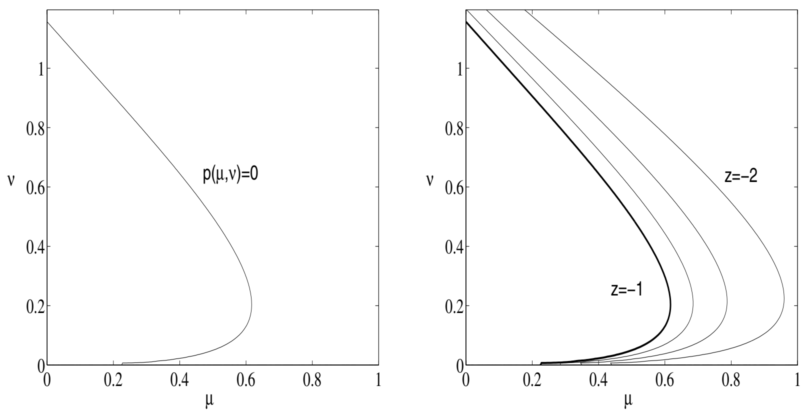
Let $p(\mu,\nu) = C(-1,\mu,\nu)$. We plot $p(\mu,\nu)=0$ in Fig. 1. a).

For (μ,ν) such that $p(\mu,\nu)<0$ there exists an eigenmode $z_{\mu\nu} < -1$ such that $C(z_{\mu\nu},\mu,\nu)=0$ (Fig. 1.b)).

This means that for $S_1 = \{(\mu,\nu) : p(\mu,\nu) < 0\}$ there exists $z_{\mu\nu}$ real and less than -1 such that $k_1(z_{\mu\nu},\mu,\nu)$ and $k_2(z_{\mu\nu},\mu,\nu)$ are solutions of f and verify (22). To assure that this eigenmode $z_{\mu\nu}$ which absolute value is bigger than one, determine an instable region we still need to verify that for these (μ,ν) we do have $|k_i(z_{\mu\nu},\mu,\nu)|<1, i=1,2$.

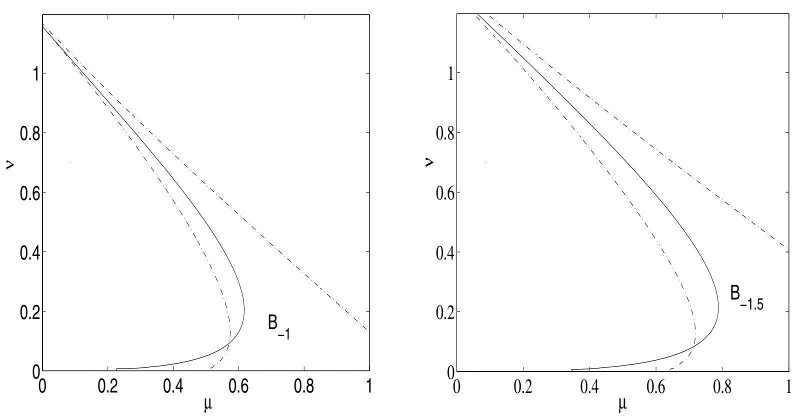
For z fixed let us define the following sets: $A_z = \{(\mu,\nu) : |k_1(z,\mu,\nu)|<1\}$ and $B_z = \{(\mu,\nu) : |k_2(z,\mu,\nu)|<1.\}$ For $z<-1$, $B_z \subset A_z$, i. e., if $|k_2(z,\mu,\nu)|<1$ then $|k_1(z,\mu,\nu)|<1$. We plot $C(z,\mu,\nu)=0$ and B_z for $z=-1,-1.5$ in Fig. 2.

From the figure we observe that in the region B_{-1} the root $k_2(-1,\mu,\nu)$, for $(\mu,\nu) : p(-1,\mu,\nu)=0$, become bigger than one approximately for $\nu<0.09$. For $z=-1.5$ the same happens but for ν even smaller. Since one of the roots we found become larger than one we can not conclude anything about the instability of the method for $\nu<0.09$. This is not a big problem since the von Neumann condition give us a stability limit for this region. We will plot the curve $p(\mu,\nu)=$



a) b)

Fig. 1. a) $p(\mu, \nu) = 0$; b) $C(z, \mu, \nu) = 0$ for $z = -1, -1.2, -1.5, -2$



a) b)

Fig. 2. a) $C(-1, \mu, \nu) = 0$ is the line (–) and B_{-1} is the region between the lines (-·-); b) $C(-1.5, \mu, \nu) = 0$ is the line (–) and $B_{-1.5}$ is the region between the lines (-·-)

0 for $\nu > 0.09$ and the von Neumann stability condition. We can see the unstable region plotted in Fig. 3. In fact running experiments numerically the region called stable in Fig. 3 is the exact region of practical stability.

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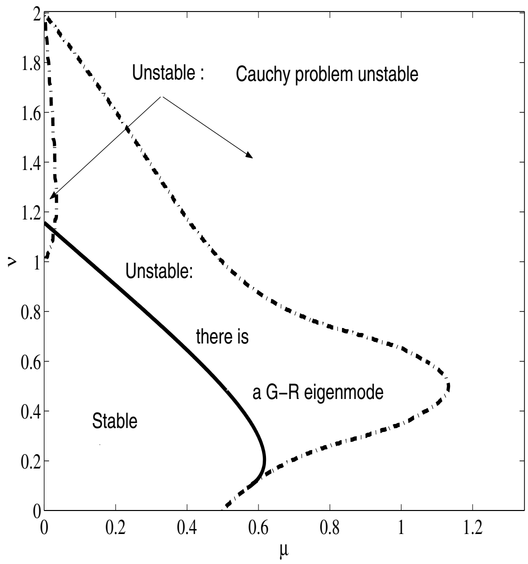

Fig. 3. Stability region: von Neumann condition (-·-) and Godunov-Ryabenkii condition (–)

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