Stability conditions for the convection-diffusion equation using the SHK Runge-Kutta method

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1 Introduction

Because numerical stability looms large in the oeuvre of Piet van der Houwen, I thought he might find the following note of interest. In [8] a system of three-dimensional convection-diffusion-reaction equations is considered, that describes transport of salinity, pollutants, suspended materical etc. This is a fairly large paper, covering many aspects, such as fractional step methods and stabilized Runge-Kutta methods. One of these Runge-Kutta methods seems particularly attractive for convection dominated problems. Let us call this the SHK Runge-Kutta method, with reference to the surnames of the authors. In the following, a handy technique to derive von Neumann stability conditions is presented and applied to the SHK Runge-Kutta method.

2 Discretization

To make von Neumann stability analysis applicable, we simplify the equations considered in [8] to the constant coefficients convection-diffusion equation:

$$\frac{\partial \varphi}{\partial t} + L\varphi = 0 \ , \quad L\varphi = \sum_{\alpha=1}^{m} (u_\alpha \frac{\partial}{\partial x_\alpha} - \varepsilon \frac{\partial^2}{\partial x_\alpha^2})\varphi \ ,$$

with m the number of space dimensions. Assuming a uniform grid, we discretize the Laplacian in the usual way and use the κ-scheme for convection, and obtain the following semi-discretized system:

$$\frac{d\varphi_j}{dt} + L_h \varphi_j = 0 \ , \quad L_h = (C_h + D_h)/\tau \ ,$$

with τ the time step (to be used later), $j = (j_1, ..., j_m)$, $j_\alpha \in \{0, \pm 1, \pm 2, ...\}$, and

$$C_h = \frac{1}{4} \sum_\alpha c_\alpha [(1-\kappa)\varphi_{j-2e_\alpha} - (5-3\kappa)\varphi_{j-e_\alpha} + (3-3\kappa)\varphi_j + (1+\kappa)\varphi_{j+e_\alpha}] \ ,$$
$$D_h = \frac{1}{2} \sum_\alpha d_\alpha (-\varphi_{j-e_\alpha} + 2\varphi_j - \varphi_{j+e_\alpha}) \ ,$$

where $e_1 = (1, 0, ..., 0)$, $e_2 = (0, 1, 0, ..., 0)$ etc., and

$$c_\alpha = u_\alpha \tau / h_\alpha \ , \quad d_\alpha = 2\varepsilon\tau / h_\alpha^2 \ ,$$

with h_α the mesh size in the x_α-direction. Here we assume $u_\alpha \geq 0$; the contrary case may be treated by symmetry. The dimensionless numbers c_α and d_α are called the Courant-Frederichs-Levy (CFL) and diffusion numbers, respectively. The scheme studied in [8] employs the second order central scheme for convection, which corresponds to $\kappa = 1$. For $-1 \leq \kappa < 1$ an upwind bias is obtained.

3 Properties of the symbol

With von Neumann stability analysis, one postulates

$$\varphi_j(t) = b(t)e^{ij\theta} , \quad j\theta = j_1\theta_1 + \cdots + j_m\theta_m , \quad 0 \le \theta_\alpha < 2\pi .$$

One finds

$$\frac{db}{dt} = -\hat{L}_h(\theta)b , \quad \hat{L}_h(\theta) = e^{-ij\theta} L_h e^{ij\theta} ,$$

where $\hat{L}_h$ is called the symbol of L_h. Discretization is completed by introducing a time stepping method, resulting in a sequence $b^0, b^1, ...$, with b^n an approximation to $b(n\tau)$, with τ the time step, assumed constant. The scheme is called stable if $\{|b^n|\}$ is non-increasing. For the symbol we find

$$\begin{aligned}
&\tau\hat{L}_h = \hat{C}_h + \hat{D}_h , \\
&\hat{C}_h(\theta) = \gamma_1(\theta) + i\gamma_2(\theta) , \quad \hat{D}_h(\theta) = \delta(\theta) , \\
&\gamma_1(\theta) = 2(1-\kappa)\sum_\alpha c_\alpha s_\alpha^2 , \quad \gamma_2(\theta) = \sum_\alpha c_\alpha\{(1-\kappa)s_\alpha + 1\}\sin\theta_\alpha , \\
&\delta(\theta) = 2\sum_\alpha d_\alpha s_\alpha , \quad s_\alpha = \sin^2 \tfrac{1}{2}\theta_\alpha .
\end{aligned}$$

The stability domain S of time stepping methods for the differential equation $dy/dt = \lambda y, \ \lambda \in \mathbb{C}$ (the complex plane) is defined as

$$S = \{\lambda\tau \in \mathbb{C} : \{|y^n| \text{ is not increasing}\} .$$

This leads to the stability condition that we will use:

$$S_L \subseteq S , \quad S_L \equiv \{-\tau\hat{L}_h(\theta) : \forall\theta\} .$$

The stability domain S is easy to come by, as shown in textbooks such as [3], [4]. For the SHK method S is shown in Fig. 1. Because of symmetry with respect to the real axis, only the upper half is shown. But it is hard to get a grip on S_L. Usually, the property $S_L \subseteq S$ is studied directly for a particular time stepping method, giving results only for that method. For another time stepping method, the analysis has to be redone completely. Our strategy here is to first derive some properties of S_L, which can then be reused in the stability analysis of various time stepping methods.

First, we take an easy case. With the central scheme for convection and no diffusion we obviously have

Property 1 If $\kappa = 1$ and $\varepsilon = 0$ then

$$S_L = \{z = iy, \quad y \in [-\sum_\alpha c_\alpha, \sum_\alpha c_\alpha]\}$$

This means that S_L is a segment of the imaginary axis.

For $\kappa \neq 1$ and/or $\varepsilon \neq 0$, S_L is hard to determine exactly, but we can give some inclusions. In [9] the following is shown, with $\tilde{d}_\alpha \equiv d_\alpha + (1-\kappa)c_\alpha, \ \tilde{d} \equiv \sum_\alpha \tilde{d}_\alpha$:

Property 2 If

$$\tilde{d} \le \frac{a}{2} \quad \text{and} \quad \sum_\alpha c_\alpha \le b/(2-\kappa)$$

then S_L is contained in the rectangle defined by

$$-a \le v \le 0 \,, \quad |w| \le b \,, \quad v + iw = z \,.$$

The first condition is necessary.

Property 3 If

$$\tilde{d} \le \frac{a}{2} \quad \text{and} \quad \frac{2\tilde{d}}{b^2} \sum_\alpha c_\alpha^2/\tilde{d}_\alpha \le (2-\kappa)^{-2}(1 + \sqrt{1 - 4\tilde{d}^2/a^2})$$

then S_L is contained in the left half of the ellipse given by

$$(v/a)^2 + (x/b)^2 = 1 \,, \quad v + iw = z \,.$$

The first condition is necessary.

These properties can be used to derive stability conditions. More such properties are given in [9], but these are not useful for deriving stability conditions for the SHK Runge-Kutta method. However, for other time stepping methods, especially if S does not contain a segment of the imaginary axis, the geometric figures of Fig. 1 (half ellipse and rectangle) do not fit inside S. For such cases, similar properties as above are derived for other geometric figures in [9].

Here we include a proof of Property 3; it is much easier to prove Property 2. Necessity of the first condition follows by taking $\theta_1 = ... = \theta_m = \pi$. We continue with sufficiency. That $-\tau\hat{L}_h$ is not in the right half of the ellipse follows from $\delta + \gamma_1 \ge 0$. It reamains to show that

$$\left(\frac{\delta + \gamma_1}{a}\right)^2 + \left(\frac{\gamma_2}{b}\right)^2 \le 1 \,.$$

Writing $\tilde{c}_\alpha = (1-\kappa)c_\alpha$ for brevity, since $0 \le s_\alpha \le 1$ we have

$$(\delta + \gamma_1)^2 = 4[\sum_\alpha (d_\alpha s_\alpha + \tilde{c}_\alpha s_\alpha^2)]^2 \le 4[\sum_\alpha \tilde{d}_\alpha s_\alpha]^2 \,.$$

Since $\tilde{d}_\alpha \ge 0$ we may write $\tilde{d}_\alpha s_\alpha = \sqrt{\tilde{d}_\alpha}(s_\alpha \sqrt{\tilde{d}_\alpha})$. The Schwartz inequality gives

$$(\delta + \gamma_1)^2 \le 4\tilde{d} \sum_\alpha \tilde{d}_\alpha s_\alpha^2 \,. \tag{1}$$

Furthermore, writing $\bar{\kappa} = 1 - \kappa$ for brevity, we have

$$\gamma_2^2 = [\sum_\alpha (c_\alpha/\sqrt{\tilde{d}_\alpha})\{\sqrt{\tilde{d}_\alpha}(\bar{\kappa}s_\alpha + 1)\sin\theta_\alpha\}]^2 \,.$$

By applying Schwartz we obtain, noting that $\sin^2\theta_\alpha = 4s_\alpha^2(1 - s_\alpha^2)$,

$$\gamma_2^2 \le 4 \sum_\alpha c_\alpha^2/\tilde{d}_\alpha \sum_\alpha \tilde{d}_\alpha s_\alpha (1 - s_\alpha)(\bar{\kappa}s_\alpha + 1)^2) \,.$$

Since $|s_\alpha| \le 1$ it follows that

$$\gamma_2^2 \le 4(2-\kappa)^2 \sum_\alpha c_\alpha^2/\tilde{d}_\alpha \sum_\alpha \tilde{d}_\alpha s_\alpha (1-s_\alpha) \ .$$

By using the second condition of Property 3 we rewrite this as

$$\left(\frac{\gamma_2}{b}\right)^2 \le \frac{4\tilde{d}}{a^2} p \sum_\alpha \tilde{d}_\alpha s_\alpha (1-s_\alpha) \ , \quad p = \tfrac{a^2}{2\tilde{d}^2}(1+\sqrt{1-4\tilde{d}^2/a^2}) \ . \tag{2}$$

Combination of (1) and (2) gives

$$\left(\frac{\delta+\gamma_1}{a}\right)^2 + \left(\frac{\gamma_2}{b}\right) \le \frac{4\tilde{d}}{a^2} \sum_\alpha \tilde{d}_\alpha s_\alpha [s_\alpha + p(1-s_\alpha)] \ .$$

Since $p \ge 2$, $\max\{s(s+p(1-s) : 0 \le s \le 1\} = p^2/[4(p-1)] = a^2/(4\tilde{d}^2)$, so that

$$\left(\frac{\delta+\gamma_1}{a}\right) + \left(\frac{\gamma_2}{b}\right) \le 1$$

and the proof is completed.

4 Stability conditions

The SHK Runge-Kutta method applied to $dy/dt = \lambda y$ is given by

$$\begin{aligned} y^* &= y^n + \frac{1}{4} z y^n \ , \\ y^{**} &= y^n + \frac{1}{3} z y^* \ , \\ y^{***} &= y^n + \frac{1}{2} z y^{**} \ , \\ y^{n+1} &= y^n + z y^{***} \ , \end{aligned}$$

where $z = \lambda\tau$. This gives

$$y^{n+1} = P(z) y^n \ , \quad P(z) = 1 + z(1 + \frac{1}{2} z(1 + \frac{1}{3} z(1 + \frac{1}{4} z))) \ .$$

The stability domain S is given by

$$S = \{z \in \mathbb{C} : |P(z)| \le 1\} \ ,$$

and is depicted in Fig. 1. Since $|P(i\sqrt{8})| = 1$, ∂S intersects the imaginary axis in $z = i\sqrt{8}$. In the case $\kappa = 1$, $\varepsilon = 0$ the stability condition $S_L \subseteq S$ gives with Property 1

$$\sum_\alpha c_\alpha \le \sqrt{8} \ ,$$

which gives the following time step restriction:

$$\tau \le \sqrt{8} / \sum_\alpha u_\alpha / h_\alpha \ .$$

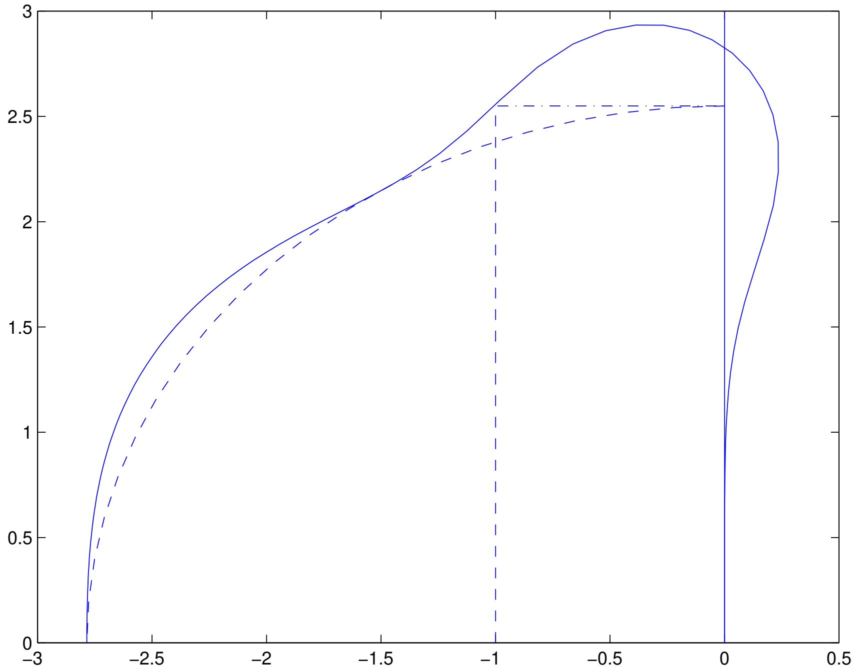

Figure 1: Stability domain of SHK Runge-Kutta method with ellipse and rectangle

This condition is also given in [8]. From the derivation it follows that this condition is necessary and sufficient. With Properties 2 and 3 we can also handle the more general case. By trial and error we find that the rectangle of Property 2 is inside S if $a = 1,\ b = 2.55$, and the ellipse of Property 3 is inside S if $a = 2.7853,\ b = 2.55$; see Fig. 1. Property 2 gives us the following stability condition:

$$\tilde{d} \le \frac{1}{2} \quad \text{and} \quad \sum_\alpha c_\alpha \le 2.55/(2-\kappa)\ ,$$

This results in the following time step restriction:

$$\begin{aligned} \tau &\le \tau_1 \quad \text{and} \quad \tau \le \tau_2\ , \\ \tau_1 &= \{2\varepsilon \sum_\alpha [(2+(1-\kappa)p_\alpha)h_\alpha^{-2}]\}^{-1}\ , \quad p_\alpha = u_\alpha h_\alpha/\varepsilon\ , \\ \tau_2 &= 2.55\{(2-\kappa)\sum_\alpha u_\alpha/h_\alpha\}^{-1}\ . \end{aligned} \tag{3}$$

Property 3 gives the following time step restriction:

$$\tau \le \tau_3 \quad \text{and} \quad \tau \le \tau_4\ , \tag{4}$$

with $\tau_3 = 2.7853\tau_1$ and

$$\tau_4 = \frac{2.55}{(2-\kappa)}\{2\sum_\alpha[(2+(1-\kappa)p_\alpha)/h_\alpha^2]\sum_\alpha[u_\alpha^2/(2+(1-\kappa)p_\alpha)]\}^{-1/2}\ ,$$

where we are a bit conservative by neglecting the factor $1+\sqrt{1-4\tilde{d}^2/a^2}$ for simplicity. Although it is easy to check in practice whether a given time step τ satisfies one of the (sufficient) stability conditions (3) or (4), the expressions for $\tau_1, ..., \tau_4$ are a bit complicated. But in one space dimension simplification occurs. One obtains

$$\begin{aligned} \tau_1 &= h^2/[4\varepsilon + (2-2\kappa)uh] , \\ \tau_2 &= 2.55h/[(2-\kappa)u] , \quad \tau_4 = \tau_2/\sqrt{2} . \end{aligned}$$

Conditions (3) and (4) are merely sufficient, and it is not known how conservative they are. Partly this depends on the degree to which the geometric figures chosen (rectangle and half ellipse in the present case) fill out S, but the question remains: how conservative are Properties 3 and 4? Here we will not go into this further.

5 Final remarks

The lack of sufficient stability conditions for many frequently used numerical schemes for partial differential equations is surprising. Often, practitioners proceed by trial and error, sometimes guided by necessary conditions derived from evaluation of the symbol for special values of the Fourier wave numbers. The technique described above makes it easy to derive sufficient stability conditions for the convection-diffusion equation with general time stepping methods. Our technique is, however, not applicable to mixed schemes, where different terms are disretized in time with different methods, for example, diffusion implicit, convection explicit. But in special circumstances, for instance, when the symbol of the convection discretization is purely imaginary, the approach described is applicable to mixed schemes; see [9]. This includes mixed schemes used for large-eddy simulation of turbulent flows, such as the leapfrog-Euler method ([1], [2], [7]) or the Adams-Bashfort-Euler method ([5]).

The essential simplifying feature of our approach lies in the fact, that we do not prove that the geometric figures selected (such as the rectangle for Property 2 and the half ellipse for Property 3) are included in the stability domain S, but allow ourselves to be satisfied by visual inspection of Fig. 1. Rigorous proofs, such as those using Schur-Cohn theory for multistep methods ([6]) are more difficult. For every multistep method one has to start from scratch, and the complexity of the analysis increases rapidly with the order of the multistep method. Our approach does not get more complicated as the order of the method increases, and applies equally to Runge-Kutta methods, because all that is needed is a picture of the stability domain. Applications to numerical schemes frequently used in computational fluid dynamics are given in [10].

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