DELFT UNIVERSITY OF TECHNOLOGY

REPORT 95-48

Von Neumann stability conditions
for the convection-diffusion equation

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ISSN 0922-5641

Reports of the Faculty of Technical Mathematics and Informatics no. 95-48

Delft 1995

Abstract

A method is presented to easily derive von Neumann stability conditions for a wide variety of time discretization schemes for the convection-diffusion equation. Spatial discretization is by the κ-scheme or the fourth order central scheme. The use of the method is illustrated by application to multistep, Runge-Kutta and implicit-explicit methods, such as are in current use for flow computations, and for which, with few exceptions, no sufficient von Neumann stability results were available.

1 Introduction

Stability criteria for the instationary convection-diffusion equation often result immediately in stability conditions for numerical methods to compute instationary incompressible flows, if the widely used pressure-correction method ([3], [15]) is applied. This is because for the velocity prediction step something very close to the convection-diffusion equation is solved, and stability analysis boils down to stability analysis for the convection-diffusion equation, which is the topic of this paper. Here, by stability we will mean stability in the sense of von Neumann, i.e. non-growth of Fourier components in the frozen coefficients case on an unbounded domain. Strictly speaking, an $O(\Delta t)$ growth per time step could be allowed, but this hardly affects the stability conditions that result.

We will present a method that is both simple and applicable to a wide variety of schemes and that gives stability conditions that are easily evaluated and not too conservative. The method has been outlined before in [18] for central discretization, using a second or a fourth order scheme for the convection term. Here the κ-scheme ([16]) will be used for the convection term. Time discretizations will be considered that are often employed for instationary incompressible flow computations, such as large-eddy or direct simulation of turbulence. No rigorous von Neumann stability conditions seem to have been derived before for these schemes.

2 Fourier stability analysis

The convection-diffusion equation is given by

$$\frac{\partial\varphi}{\partial t} + L\varphi = 0, \quad L\varphi = \sum_{\alpha=1}^{m}(u_\alpha \frac{\partial}{\partial x_\alpha} - \nu \frac{\partial^2}{\partial x_\alpha^2})\varphi \tag{2.1}$$

with m the number of dimensions. For Fourier stability analysis, u_α and ν are taken constant, and the domain is unbounded. With the κ-scheme, the discretization of L on a uniform grid with mesh-sizes $h_1, ..., h_m$ is given by $L_h = C_h + D_h$ with

$$C_h = \frac{1}{4\tau}\sum_\alpha c_\alpha\{(1-\kappa)\varphi_{j-2e_\alpha} - (5-3\kappa)\varphi_{j-e_\alpha} + (3-3\kappa)\varphi_j + (1+\kappa)\varphi_{j+e_\alpha}\} \tag{2.2}$$

and

$$D_h = \frac{1}{2\tau}\sum_\alpha d_\alpha(-\varphi_{j-e_\alpha} + 2\varphi_j - \varphi_{j-e_\alpha}) \tag{2.3}$$

where $j = (j_1, ..., j_m)$, $e_1 = (1, 0, ..., 0)$, $e_2 = (0, 1, 0, ..., 0)$ etc., and

$$c_\alpha = u_\alpha\tau/h_\alpha\ , \quad d_\alpha = 2\nu\tau/h_\alpha^2 \tag{2.4}$$

with τ the time step. The dimensionless numbers c_α and d_α, called the Courant and diffusion numbers, respectively, govern stability. In (2.2), $u_\alpha \geq 0$ has been assumed; the contrary case may be treated by symmetry. For $\kappa = -1$ we have the one-sided fully upwind scheme ([13]). With $\kappa = 0$ one obtains Fromm's zero average phase error scheme ([4]), if the terms quadratic in the Courant number are neglected, which are meant to improve time accuracy; this scheme results by optimizing, among 5-point schemes, for the propagation of a step function over one time step in the absence of diffusion ([17]). For $\kappa = 1/3$ the third order upwind biased scheme ([1]) results. For $\kappa = 1/2$ we have the second order QUICK (quadratic upstream interpolation for convective kinematics) scheme proposed in [7]. Finally, $\kappa = 1$ gives the central second order scheme.

A fourth order central discretization of the convection term is given by

$$C_h = \frac{1}{12\tau}\sum_\alpha c_\alpha(\varphi_{j-2e_\alpha} - 8\varphi_{j-e_\alpha} + 8\varphi_{j+e_\alpha} - \varphi_{j+2e_\alpha}) \tag{2.5}$$

First order upwind discretization is included in the analysis that follows by taking $\kappa = 1$ and redefining $d_\alpha = d_\alpha + |c_\alpha|$.

After spatial discretization we are left with the following system of ordinary differential equations:

$$d\varphi/dt = -L_h\varphi_j \tag{2.6}$$

The symbol or Fourier transform $\hat{L}_h(\theta)$ of L_h is defined by $\hat{L}_h(\theta) = e^{-ij\theta}L_h e^{ij\theta}$ with $\theta = (\theta_1, ..., \theta_m)$. One finds:

$$\begin{aligned} \tau\hat{L}_h(\theta) &= \hat{C}_h(\theta) + \hat{D}_h(\theta) \\ \tau\hat{C}_h(\theta) &= \gamma_1(\theta) + i\gamma_2(\theta), \quad \hat{D}_h(\theta) = \delta(\theta) \end{aligned} \tag{2.7}$$

For (2.2) we have

$$\gamma_1(\theta) = 2(1-\kappa)\sum_\alpha |c_\alpha| s_\alpha^2\ , \quad \gamma_2(\theta) = \sum_\alpha c_\alpha\{(1-\kappa)s_\alpha + 1\}\sin\theta_\alpha \tag{2.8}$$

where $s_\alpha = \sin^2\frac{1}{2}\theta_\alpha$, whereas for (2.5)

$$\gamma_1(\theta) = 0\ , \quad \gamma_2(\theta) = \frac{1}{6}\sum_\alpha c_\alpha(8\sin\theta_\alpha - \sin 2\theta_\alpha) \tag{2.9}$$

Furthermore,

$$\delta(\theta) = 2\sum_\alpha d_\alpha s_\alpha \tag{2.10}$$

For Fourier (or von Neumann) stability analysis one substitutes $\varphi_j(t) = y(t)e^{ij\theta}$ in (2.6), and obtains

$$dy/dt = -\hat{L}_h(\theta)y \tag{2.11}$$

Sufficient for von Neumann stability is

$$S_L \subseteq S, \quad S_L = \{-\tau\hat{L}_h(\theta) \in \mathbb{C} : \forall\theta\} \tag{2.12}$$

with S the stability domain of the time discretization method to be used.

3 Some useful theorems

For the derivation of sufficient stability conditions, the following theorems, which form the substance of our method, are useful. But first some preliminaries. The κ-scheme (2.2), (2.3) will be called scheme 1 and (2.3), (2.5) will be called scheme 2. Define $\tilde{c}_\alpha = (1-\kappa)|c_\alpha|$ for scheme 1 and $\tilde{c}_\alpha = 0$ for scheme 2. Let $\tilde{d}_\alpha = d_\alpha + \tilde{c}_\alpha$ and $\tilde{d} = \sum_\alpha \tilde{d}_\alpha$. Schwarz's inequality will be used frequently. For schemes 1 and 2 we have

$$(\delta + \gamma_1)^2 = 4\{\sum_\alpha d_\alpha s_\alpha + \tilde{c}_\alpha s_\alpha^2\}^2 \leq 4\{\sum_\alpha \tilde{d}_\alpha s_\alpha\}^2 \leq 4\tilde{d}\sum_\alpha \tilde{d}_\alpha s_\alpha^2 \tag{3.1}$$

Furthermore, for scheme 1,

$$\gamma_2^2 \leq 4\sum_\alpha c_\alpha^2/d_\alpha \sum_\alpha d_\alpha s_\alpha(1-s_\alpha)(\bar{\kappa}s_\alpha + 1)^2 \tag{3.2}$$

where $\bar{\kappa} = 1-\kappa$, whereas for scheme 2 we find that (3.2) holds with $\kappa = 1/3$. From (3.2) it follows that

$$\gamma_2^2 \leq 4(2-\kappa)^2 \sum_\alpha c_\alpha^2/d_\alpha \sum_\alpha d_\alpha s_\alpha(1-s_\alpha) \tag{3.3}$$

Similarly, for scheme 1,

$$\begin{aligned} \gamma_2^4 &\leq \{\sum_\alpha (|c_\alpha|^{2/3} d_\alpha^{-1/6})|c_\alpha|^{1/3} d_\alpha^{1/6}(\bar{\kappa}s_\alpha + 1)|\sin\theta_\alpha|\}^4 \\ &\leq 16\{\sum_\alpha (c_\alpha^4/d_\alpha)^{1/3}\}^3 \sum_\alpha d_\alpha(\bar{\kappa}s_\alpha+1)^4 s_\alpha^2(1-s_\alpha)^2 \end{aligned} \tag{3.4}$$

which also holds for scheme 2 with $\kappa = 1/3$. For arbitrary $a > 0$ we have for schemes 1 and 2

$$(\frac{\delta+\gamma_1}{a} - 1)^2 \leq 1 + \frac{4\tilde{d}}{a^2}\sum_\alpha \tilde{d}_\alpha s_\alpha^2 - \frac{4}{a}\sum_\alpha (d_\alpha s_\alpha + \tilde{c}_\alpha s_\alpha^2) \tag{3.5}$$

If $\tilde{d} \leq a$ this gives

$$(\frac{\delta+\gamma_1}{a} - 1)^2 \leq 1 + \frac{4}{a}\sum_\alpha d_\alpha(s_\alpha^2 - s_\alpha) \tag{3.6}$$

Theorem 3.1 *If*

$$\tilde{d} \leq a \quad and \quad \sum_\alpha c_\alpha^2/d_\alpha \leq (2-\kappa)^{-2} b^2/a \tag{3.7}$$

then for scheme 1 S_L is contained in the ellipse

$$(v/a+1)^2 + (w/b)^2 = 1\,, \quad v + iw = z \tag{3.8}$$

The first condition is necessary.

Proof

Necessity of the first condition follows by taking $s_\alpha = 1$, $\alpha = 1, ..., m$. It remains to show that $\{(\delta + \gamma_1)/a - 1\}^2 + (\gamma_2/b)^2 \leq 1$. Using (3.3), (3.6) and (3.7) we have

$$(\frac{\delta+\gamma_1}{a} - 1)^2 + (\frac{\gamma_2}{b})^2 \leq 1 + \frac{4}{a}\sum_\alpha d_\alpha s_\alpha (1 - s_\alpha)(-1+1) \leq 1$$

and the proof is completed.

For $\kappa = 1$ necessity of both conditions is shown in [18]. The conditions (3.7) are equivalent to

$$\tau \leq \min\{a/\sum_\alpha (2\nu h_\alpha^{-2} + (1-\kappa)|u_\alpha| h_\alpha^{-1}),\ 2\nu(2-\kappa)^{-2}\frac{b^2}{a}/\sum_\alpha u_\alpha^2\} \tag{3.9}$$

Theorem 3.2 *If*

$$\tilde{d} \leq a \tag{3.10}$$

and one or both of the following two conditions hold:

$$\sum_\alpha (c_\alpha^4/d_\alpha)^{1/3} \leq q_1 (b^4/a)^{1/3} \quad or \quad \sum_\alpha |c_\alpha| \leq q_2 b^2/a \tag{3.11}$$

where

$$\begin{aligned}
q_1 &= \frac{1}{4}(8-4\kappa)^{-5/3}(15-5\kappa-r)^{4/3}(5\kappa-3+r)^{1/3}(9-7\kappa+r)^{1/3}\,, \\
r &= (25\kappa^2 - 54\kappa + 33)^{1/2}\,, \\
q_2 &= (1-\kappa)^{3/2}(8/5 - 4\kappa/5)^{-5/2}\,,\ -1 \leq \kappa < 3/4\,, \\
q_2 &= (1-\kappa)/2\,,\ 3/4 \leq \kappa \leq 1
\end{aligned}$$

then for scheme 1 S_L is contained in the oval given by

$$(v/a+1)^2 + (w/b)^4 = 1\,, \quad v + iw = z \tag{3.12}$$

Condition (3.10) is necessary.

Proof

Necessity of (3.10) follows by taking $s_\alpha = 1$, $\alpha = 1, ..., m$. Next, assume that (3.10) and the first condition of (3.11) hold. Using (3.4) and (3.6),

$$(\frac{\delta+\gamma_1}{a} - 1)^2 + (\frac{\gamma_2}{b})^4 \leq 1 + \frac{4}{a}\sum_\alpha d_\alpha (s_\alpha - s_\alpha^2)\{-1 + 4q_1^3(\bar{\kappa} s_\alpha + 1)^4 s_\alpha (1 - s_\alpha)\} \tag{3.13}$$

We have

$$\max\{(\bar\kappa s+1)^4 s(1-s):\ 0\le s\le 1\} = 1/4q_1^3$$

Hence, no term in the sum in (3.13) is positive, so that

$$(\frac{\delta+\gamma_1}{a}-1)^2+(\frac{\gamma_2}{b})^4 \le 1 \tag{3.14}$$

Next, assume that (3.10) and the second condition of (3.11) hold. Because of (3.10), $0 \le \delta+\gamma_1 \le 2a$, hence

$$\begin{aligned}
(\frac{\delta+\gamma_1}{a}-1)^2 &= \frac{\delta}{a}(\frac{\delta+\gamma_1}{a}+\frac{\gamma_1}{a}-2)+(\frac{\gamma_1}{a}-1)^2\\
&\le (\frac{\delta}{a}-2)\frac{\gamma_1}{a}+(\frac{\gamma_1}{a})^2+1)\\
&\le (2\frac{\tilde d}{a}-2-\frac{2}{a}\sum_\alpha \tilde c_\alpha)\frac{2}{a}\sum_\alpha \tilde c_\alpha s_\alpha^2+\frac{4}{a^2}\sum_\alpha \tilde c_\alpha \sum_\alpha \tilde c_\alpha s_\alpha^4+1\\
&\le 1-\frac{4\tilde c}{a^2}\sum_\alpha \tilde c_\alpha(s_\alpha^2-s_\alpha^4)
\end{aligned}$$

where $\tilde c=\sum_\alpha \tilde c_\alpha$. Furthermore, similar to (3.4),

$$\begin{aligned}
\gamma_2^4 &\le 16\{\sum_\alpha (c_\alpha^4/\tilde c_\alpha)^{1/3}\}^3\sum_\alpha \tilde c_\alpha(\bar\kappa s_\alpha+1)^4 s_\alpha^2(1-s_\alpha)^2\\
&= \frac{16}{\bar\kappa}\{\sum_\alpha |c_\alpha|\}^3\sum_\alpha \tilde c_\alpha(\bar\kappa s_\alpha+1)^4 s_\alpha^2(1-s_\alpha)^2
\end{aligned}$$

Hence

$$(\frac{\delta+\gamma_1}{a}-1)^2+(\frac{\gamma_2}{b})^4 \le 1+\frac{4\tilde c}{a^2}\sum_\alpha \tilde c_\alpha s_\alpha^2(1-s_\alpha)\{\frac{4q_2^2}{\bar\kappa^2}(\bar\kappa s_\alpha+1)^4(1-s_\alpha)-s_\alpha-1\}$$

Observing that

$$\max\{(\bar\kappa s+1)^4(1-s):\ 0\le s\le 1\,,\ 0\le\bar\kappa\le 2\} = \bar\kappa^2/4q_2^2$$

we see that each term in the preceding sum is non-positive, hence (3.14) holds, and the proof is completed.

Note that the first condition of (3.11) is not useful in the hyperbolic case ($\nu=0$, i.e. $d_\alpha=0$), whereas the second condition is not useful for $\kappa=1$; the two conditions complement each other.

Conditions (3.10) and (3.11) are equivalent to

$$\begin{aligned}
\tau &\le a/\sum_\alpha(2\nu h_\alpha^{-2}+(1-\kappa)|u_\alpha|h_\alpha^{-1}) \quad\text{and}\\
\tau &\le \max\{q_1(\tfrac{2\nu b^4}{a})^{1/3}/\sum_\alpha(u_\alpha^4/h_\alpha^2)^{1/3}\,,\ \tfrac{q_2 b^2}{a}/\sum_\alpha|u_\alpha|h_\alpha^{-1}\}
\end{aligned} \tag{3.15}$$

Theorem 3.3 *If*

$$\tilde{d} \leq \frac{a}{2} \quad and \quad \frac{2\tilde{d}}{b^2}\sum_\alpha c_\alpha^2/\tilde{d}_\alpha \leq (2-\kappa)^{-2}(1+\sqrt{1-4\tilde{d}^2/a^2}) \tag{3.16}$$

then for scheme 1 S_L is contained in the ellipse given by

$$(v/a)^2 + (w/b)^2 = 1, \quad v + iw = z \tag{3.17}$$

The first condition is necessary.

Proof
Necessity of the first condition follows by taking $s_\alpha = 1$, $\alpha = 1, ..., m$. Using (3.1, (3.3) and (3.16) we have

$$(\frac{\delta+\gamma_1}{a})^2 + (\frac{\gamma_2}{b})^2 \leq 4\frac{\tilde{d}}{a^2}\sum_\alpha \tilde{d}_\alpha s_\alpha\{s_\alpha + p(1-s_\alpha)\}$$

where $p = (a^2/2\tilde{d}^2)(1+\sqrt{1-4\tilde{d}^2/a^2})$. Since $p > 2$, $\max\{s(s+p(1-s)) : 0 \leq s \leq 1\} = p^2/\{4(p-1)\} = a^2/(4\tilde{d}^2)$, so that

$$(\frac{\delta+\gamma_1}{a})^2 + (\frac{\gamma_2}{b})^2 \leq 1$$

and the proof is completed.

The conditions (3.16) are equivalent to

$$\begin{aligned} \tau \leq \; & \min[\frac{1}{2}a/\sum_\alpha(2\nu h_\alpha^{-2} + (1-\kappa)|u_\alpha|h_\alpha^{-1}), \\ & b(2-\kappa)^{-1}\{\sum_\alpha u_\alpha^2 \sum_\alpha(2\nu h_\alpha^{-2} + (1-\kappa)|u_\alpha|h_\alpha^{-1})\}^{-1/2}(1+\sqrt{1-4\tilde{d}^2/a^2})^{1/2}] \end{aligned} \tag{3.18}$$

This inequality is implicit, because $\tilde{d}$ depends on τ. However, checking the admissibility of a given τ is straightforward, whereas generation of a suitable τ is easily done by some iterative process.

Theorem 3.4 *If*

$$\sum_\alpha c_\alpha^2/d_\alpha \leq q_3 b^2 \tag{3.19}$$

where

$$\begin{aligned} q_3 &= 1/2 \quad if \quad 1/2 \leq \kappa \leq 1\,, \\ q_3 &= \tfrac{27}{8}(1-\kappa)/(2-\kappa)^3 \quad if \quad -1 \leq \kappa < 1/2 \end{aligned} \tag{3.20}$$

then for scheme 1 S_L is contained in the parabola given by

$$v + (w/b)^2 = 0\,, \quad v + iw = z \tag{3.21}$$

Proof
We have to show that $-\delta - \gamma_1 + (\gamma_2/b)^2 \leq 0$. Using (3.2) we have

$$-\delta - \gamma_1 + (\gamma_2/b)^2 \leq 2\sum_\alpha d_\alpha s_\alpha\{-1 + 2q_3(1-s_\alpha)(\bar{\kappa}s_\alpha + 1)^2\} \tag{3.22}$$

Observing that

$$\max\{(1-s)(\bar{\kappa}s+1)^2 : \ 0 \leq s \leq 1\} = 1/2q_3 \tag{3.23}$$

the proof is completed.

The condition (3.19) is equivalent to

$$\tau \leq 2\nu q_3 b^2 / \sum_\alpha |u_\alpha|^2 \tag{3.24}$$

For scheme 2 we have $\gamma_1 = 0$ and $\kappa = 1/3$. It is easy to see that theorems 3.1, 3.4 and 3.4 hold with $\tilde{d}$ and $\tilde{d}_\alpha$ replaced by $d = \sum_\alpha d_\alpha$ and d_α, and $\kappa = 1/3$, whereas instead of theorem 3.2 we have

Theorem 3.5 *If*

$$d \leq a \quad and \quad \sum_\alpha (c_\alpha^4/d_\alpha)^{1/3} \leq q_4(b^4/a)^{1/3} \tag{3.25}$$

with $q_4 = \frac{1}{5}(\sqrt{10}-1)^{5/3}(\frac{5+\sqrt{10}}{12})^{1/3}$ *then for scheme 2* S_L *is contained in the oval given by (3.12). The first condition of (3.25)is necessary.*

Proof
Necessity of the first part of (3.25) follows by taking $s_\alpha = 1$, $\alpha = 1, ..., m$. The remainder of the proof is the same as the proof that (3.10) and the first part of (3.11) are sufficient, by substituting $\gamma_1 = 0$ and $\kappa = 1/3$.

Conditions (3.25) are equivalent to the following restrictions on the time step τ:

$$\tau \leq \min\{\frac{a}{2\nu}/\sum_\alpha h_\alpha^{-2} \ , \ q_3(\frac{2\nu b^4}{a})^{1/3}/\sum_\alpha (u_\alpha^4/h_\alpha^2)^{1/3}\} \tag{3.26}$$

4 Von Neumann stability conditions for various time discretizations

All that remains to be done is to choose suitable unions or intersections of the sets considered in theorems 3.1-3.5 (ellipses, oval, parabola) inside the stability domain S of the time discretization method, and useful (i.e. not too conservative and easy to evaluate) sufficient conditions for von Neumann stability tumble like ripe apples. It appears that until now only in rare cases sufficient von Neumann stability conditions have been published for the explicit or implicit-explicit (IMEX: diffusion implicit, convection explicit) schemes currently used for time-dependent incompressible flow computations. In some cases necessary but not sufficient

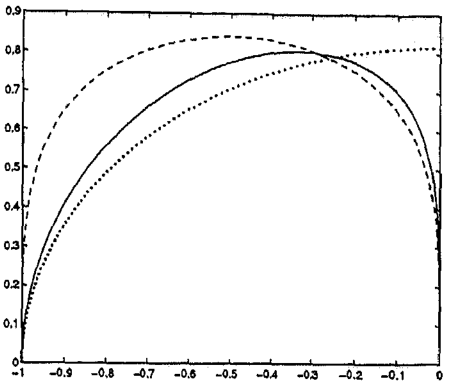

Figure 4.1: Stability domain of second order Adams-Bashforth scheme (—) with oval (- - -) and ellipse (· · ·)

conditions are known for the Courant numbers c_α. Fully implicit schemes are usually easily seen to be unconditionally stable. The techniques used to derive the preceding theorems can also be used to obtain stability conditions for cases where the ellipses, oval and/or parabola do not fit nicely in S; an example will be given. Applications will be given to schemes of current or historical interest.

Explicit Euler The stability domain S is the disk $|z+1| \leq 1$. With $a = b = 1$, theorem 3.1 immediately gives sufficient stability conditions. In the case $\kappa = 1$ (second order central scheme) these conditions are shown to be also necessary in [18], and identical to those obtained in [6], [9], [5].

Adams-Bashforth The second order Adams-Bashforth scheme has the following characteristic polynomial:

$$\xi^2 - \xi + z(\frac{3}{2}\xi - \frac{1}{2}) \tag{4.1}$$

with $z = \delta + \gamma_1 + i\gamma_2$. The boundary ∂S of the stability domain S is found by substituting $\xi = e^{i\mu}$, $0 \leq \mu < 2\pi$ and solving for $-z$; the result is shown in Figure 4.1. Only the upper half of S is shown; all stability domains to be encountered are symmetric with respect to the real axis. Near $z = 0$ we have $|\mu| \ll 1$, and on ∂S we have $w \cong \pm(-4v)^{1/4}$, $v + iw = z$. On the oval (3.12) we have $w \cong \pm c(-2v/g)^{1/4}$; $a = 1/2$ and $b = 2^{-1/4}$ result in the oval shown in Figure 4.1. Near $z = -1$ we have $\mu = \pi + \varepsilon$, $|\varepsilon| \ll 1$, and on $\partial S:\ z \cong -1+v+iw,\ w = 3\sqrt{v/5}$. On the ellipse (3.17) with $a = 1$ we have $z \cong -1+v+iw$ with $w = b\sqrt{2v}$. Choosing $b = \sqrt{2/3}$ results in the ellipse shown in Figure 4.1. Useful sufficient stability conditions are obtained by requiring $-\tau\hat{L}_h(\theta) \subseteq$ ellipse $\cap$ oval.

Combination of theorems 3.2 and 3.3 results in the following sufficient conditions for von Neumann stability for scheme 1:

$$\begin{aligned} &\tilde{d} \leq 1/2 \quad \text{and} \quad 3\tilde{d}\sum_\alpha c_\alpha^2/\tilde{d}_\alpha \leq (2-\kappa)^{-2}(1+\sqrt{1-4\tilde{d}^2}) \\ &\text{and} \quad \{\sum_\alpha (c_\alpha^4/d_\alpha)^{1/3} \leq q_1 \quad \text{or} \quad \sum_\alpha |c_\alpha| \leq q_2\sqrt{2}\} \end{aligned} \tag{4.2}$$

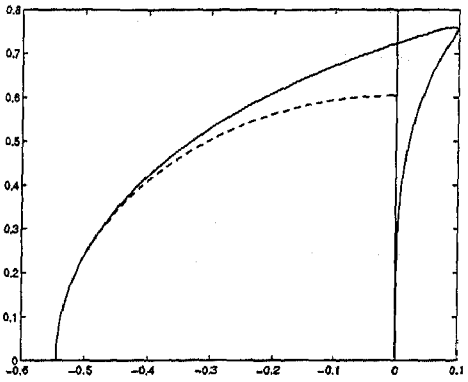

Figure 4.2: Stability domain of third order Adams-Bashforth scheme (—-) with osculating ellipse (- - -)

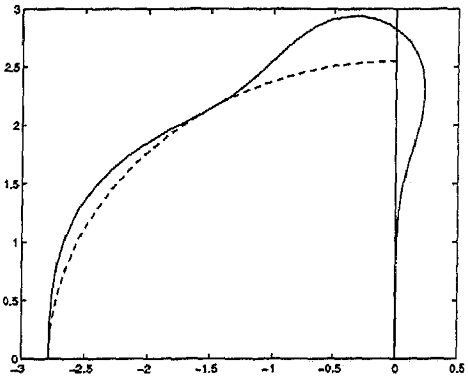

Figure 4.3: Stability domain of RK24 scheme (—-) and ellipse (- - -)

The corresponding restrictions on τ are easily found from (3.15) and (3.18) by substitution of the relevant values for a and b. Similar conditions can be obtained for scheme 2 by using theorem 3.5 instead of theorem 3.2. The third order Adams-Bashforth scheme has the following characteristic polynomial:

$$\xi^3 - \xi^2 + \frac{1}{12}z(23\xi^2 - 16\xi + 5) \tag{4.3}$$

The stability domain is given in Figure 4.2. It is covered to a satisfactory extent by the ellipse (3.17) that osculates in $z = -6/11$; its parameters are found to be $a = 6/11$, $b = \frac{72}{11}\sqrt{\frac{2}{235}} \cong 0.6038$. Theorem 3.3 immediately results in sufficient Neumann stability conditions.

Runge-Kutta To show the versatility of the method, we also apply it to a Runge-Kutta method. For a four-stage method, the amplification factor is given by

$$P(z) = 1 + z(1 + \alpha_3 z(1 + \alpha_2(1 + \alpha_1 z))) \tag{4.4}$$

In [12] a Runge-Kutta method is presented that is especially designed for convection-diffusion problems, with coefficients $\alpha_1 = 1/4,\ \alpha_2 = 1/3,\ \alpha_3 = 1$. For von Neumann stability we must have

$$|P(z)| \leq 1 \quad \text{for} \quad -z \in S_L \tag{4.5}$$

The stability domain follows from solving $|P(-2 + re^{i\mu})| = 1$ for r, while varying μ, and is given in Figure 4.3. It is covered to a satisfactory extent by the ellipse (3.17) with $a = 2.7853,\ b = 2.55$. Stability conditions follow from theorem 3.3. It seems that stability conditions for Runge-Kutta schemes applied to the convection-diffusion equation have been given in special cases only, such as for $d = 0$ and $k = 1$.

Leapfrog-Euler This is an example of a mixed scheme, in which different time discretizations are used for the convection and diffusion terms. Leapfrog is applied to the convection term, and explicit Euler to the diffusion term. The stability polynomial is given by

$$\xi^2 + 2\gamma(\theta)\xi + 2\delta(\theta) - 1 \tag{4.6}$$

with $\gamma = \gamma_1 + i\gamma_2$. For mixed methods, the coefficients of the stability polynomial and hence the location of its roots do not depend on a single complex parameter z ($z = \gamma + \delta$ in the preceding cases), so that the stability domain S is no longer a subset of the complex plane. In the case of (4.7), where δ happens to be real, the roots depend on three parameters γ_1, γ_2 and δ, and S is a subset of $I\!R^3$. It would not be difficult to re-interpret our theorems in this three-dimensional setting, but a visual check whether the sets of the theorems are contained in S is much less straightforward in three than in two dimensions. We will not do this here, and restrict ourselves for mixed schemes to the case $\gamma_1 = 0$, i.e. central second order ($\kappa = 1$) or fourth order (scheme 2) discretization of the convection term. Hence, the roots of the stability polynomial depend only on two parameters, δ and γ_2, and we can continue to work in the complex z-plane, with $z = -\delta - i\gamma_2$.

Substitution of $\xi = e^{i\mu},\ 0 \leq \mu < 2\pi$, in (4.7), equating the stability polynomial to zero and solving for $z = -\delta - i\gamma_2$ as a function of μ gives the boundary of stability domain S, the upper half of which is shown in Figure 4.4. The ellipses, oval and parabola fit badly, and we proceed directly. For von Neumann stability it is necessary and sufficient that $\delta + |\gamma_2| \leq 1$, or, for $\kappa = 1$,

$$\sum_\alpha \{d_\alpha(1 - \cos\theta_\alpha) + |c_\alpha \sin\theta_\alpha|\} \leq 1, \quad 0 \leq \theta_\alpha < 2\pi \tag{4.7}$$

Since $\theta_1, ..., \theta_m$ are independent, the maximum is obtained by maximizing each term individually. Defining $f(\theta) = d(1 - \cos\theta) + |c|\sin\theta,\ 0 \leq \theta < \pi$, we have $f'(\theta) = 0$ for $\theta = \pi - \gamma,\ \tan\gamma = |\sigma|/d,\ 0 \leq \gamma < \pi/2$, resulting in $\max\{f(\theta) : 0 \leq \theta < \pi\} = d + \sqrt{c^2 + d^2}$. This gives us the following necesary and sufficient stability condition:

$$\sum_\alpha \{d_\alpha + \sqrt{d_\alpha^2 + c_\alpha^2}\} \leq 1 \tag{4.8}$$

The one-dimensional version of this result has appeared in [2], with a less elementary proof (using Schur-Cohn theory). On heuristic grounds, the following stability condition, generally used in practice, was put forward in [11] and proved in [10] (using Schur-Cohn theory):

$$\sum_{\alpha}\{2d_\alpha + |c_\alpha|\} \leq 1 \tag{4.9}$$

We see that this condition is sufficient but not necessary. Because of trouble with spurious modes (necessitating application of the so-called Asselin filter), this scheme now seems to be less favored than Adams-Bashforth for large-eddy and direct simulation of turbulence.

For fourth order central discretization (2.5) (scheme 2) we must have:

$$\sum_{\alpha}\{d_\alpha(1-\cos\theta_\alpha) + \frac{1}{6}|c_\alpha|\ |8\sin\theta_\alpha - \sin 2\theta_\alpha|\} \leq 1, \quad 0 \leq \theta_\alpha < 2\pi \tag{4.10}$$

Since $|8\sin\theta_\alpha - \sin 2\theta_\alpha| \leq 10|\sin\theta_\alpha|$ it is sufficient if

$$\sum_{\alpha}\{d_\alpha(1-\cos\theta_\alpha) + \frac{5}{3}|c_\alpha \sin\theta_\alpha|\} \leq 1, \quad 0 \leq \theta_\alpha < 2\pi \tag{4.11}$$

Proceeding as before we find the following sufficient condition:

$$\sum_{\alpha}\{d_\alpha + \sqrt{d_\alpha^2 + \frac{25}{9}c_\alpha^2}\} \leq 1 \tag{4.12}$$

Adams-Bashforth-Crank-Nicolson This is an example of a mixed scheme of *IMEX* (implicit-explicit) type. Second order Adams-Bashforth is applied to the convection term and Crank-Nicolson to the diffusion term. The stability polynomial is given by

$$\xi^2\{1+\frac{1}{2}\delta(\theta)\} + \xi\{\frac{1}{2}\delta(\theta) + \frac{3}{2}\gamma(\theta) - 1\} - \frac{1}{2}\gamma(\theta) \tag{4.13}$$

with $\gamma = \gamma_1 + i\gamma_2$. Again, this being a mixed scheme, the roots are not a function of $z = \delta + \gamma$, but our approach still works if $\gamma_1 = 0$, in a similar way as in the preceding case. The stability domain S in the z-plane, $z = -\delta - i\gamma_2$, is plotted in Figure 4.5, together with the parabola (3.21) with $b = 2/\sqrt{3}$ and the oval (3.12) with $a = 1/2$, $b = (3/4)^{1/4}$. We have

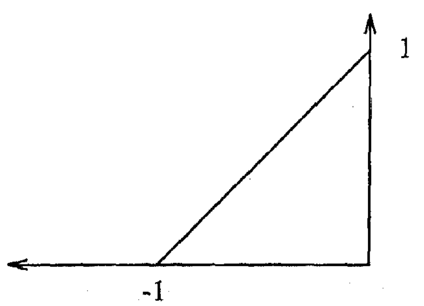

Figure 4.4: Stability domain of Leapfrog-Euler.

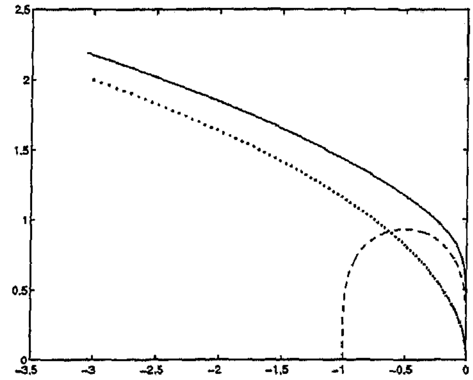

Figure 4.5: Stability domain of Adams-Bashforth-Crank-Nicolson (—-) with oval (- - -) and parabola $(\cdots)$

{parabola $\cup$ oval} $\subseteq S$, so that for $\kappa = 1$ (convection second order central) theorems 3.2 and 3.4 give the following sufficient stability conditions:

$$\{d \leq 1/2 \quad \text{and} \quad \sum_\alpha (c_\alpha^4/d_\alpha)^{1/3} \leq (3/2)^{1/3}\} \quad \text{or} \quad \sum_\alpha c_\alpha^2/d_\alpha \leq 2/3 \tag{4.14}$$

whereas for scheme 2 theorems 3.4 and 3.5 give

$$\{d \leq 1/2 \quad \text{and} \quad \sum_\alpha (c_\alpha^4/d_\alpha)^{1/3} \leq q_4(3/2)^{1/3}\} \quad \text{or} \quad \sum_\alpha c_\alpha^2/d_\alpha \leq 3^4/5^3 \tag{4.15}$$

Using Schur-Cohn theory, in [14] the following sufficient condition is derived for the one-dimensional case and $\kappa = 1 : c_1^2/d_1 \leq 1/6$, which is significantly more restrictive than (4.14); a symptom of the unwieldiness of the Schur-Cohn conditions.

Adams-Bashforth-Euler Like Adams-Bashforth, this is another scheme that tends to replace leapfrog-Euler. The convection term is treated with second order Adams-Bashforth and the diffusion term with explicit Euler. The stability polynomial is given by

$$\xi^2 - \xi + \delta(\theta)\xi + \frac{1}{2}\gamma(\theta)(3\xi - 1) \tag{4.16}$$

with $\gamma = \gamma_1 + i\gamma_2$, and again our method works only if $\gamma_1 = 0$. The stability domain S in the z-plane, $z = \delta + i\gamma_2$ is plotted in Figure 4.6. For comparison, the stability domain of second order Adams-Bashforth is also shown. The ellipse (3.17) that osculates in $z = -2$ has parameters $a = 2$, $b = 1/\sqrt{3}$. The oval in Figure 4.6 has parameters $a = b = 1$. We have {ellipse $\cap$ oval} $\subseteq S$, so that for $\kappa = 1$ theorems 3.2 and 3.3 give

$$d \leq 1 \quad \text{and} \quad \sum_\alpha (c_\alpha^4/d_\alpha)^{1/3} \leq 1 \quad \text{and} \quad d\sum_\alpha c_\alpha^2/d_\alpha \leq \frac{1}{6}(1 + \sqrt{1 - d^2}) \tag{4.17}$$

whereas for scheme 2 theorems 3.2 and 3.3 give, with $\kappa = 1/3$ and $\tilde{c}_\alpha = 0$

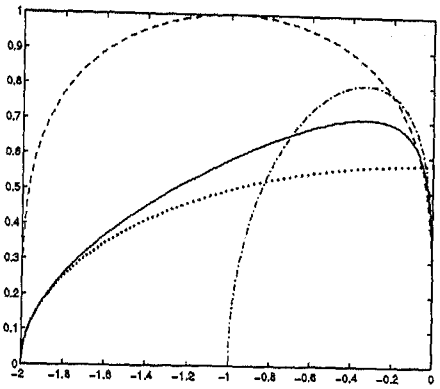

Figure 4.6: Stability domains of Adams-Bashforth-Euler (—) and second order Adams-Bashforth (– · – · –), with oval (- - -) and osculating ellipse (· · ·)

$$d \leq 1 \quad \text{and} \quad \sum_\alpha (c_\alpha^4/d_\alpha)^{1/3} \leq q \quad \text{and} \quad d\sum_\alpha c_\alpha^2/d_\alpha \leq \frac{3}{50}(1+\sqrt{1-d^2}) \tag{4.18}$$

with

$$q = \frac{1}{5}\left(\frac{5+\sqrt{10}}{12}\right)^{1/3}(\sqrt{10}-1)^{5/3} \cong 0.6360\,.$$

5 Concluding remarks

Von Neumann stability analysis for the convection-diffusion equation involves deriving conditions for the roots of the characteristic polynomial of the multistep time discretization method employed to be in the unit disk. Schur-Cohn theory, as described in [8], gives necessary and sufficient conditions on the coefficients. However, deriving stability restrictions on the time step from these conditions is usually an arduous task, that has to be undertaken anew for each scheme that one wishes to consider, and gets rapidly out of hand as the order of the multistep method increases. Hence, it is not surprising that few results have been published. Furthermore, Schur-Cohn theory is not applicable to Runge-Kutta methods, for which not the absolute value of the roots but of the characteristic polynomial itself is not to exceed 1. In the foregoing we have presented an alternative approach. Based on theorems 3.1-3.5, stability conditions are easy to find. Our approach does not get more complicated as the order of multistep methods increases, and applies equally to Runge-Kutta methods. Although not its principle, its ease of use in practice is affected if the characteristic polynomial depends on more than two parameters, so that the classical stability diagram of the time discretization method does not apply. This may happen if the terms in the partial differential equation under consideration are not all discretized in time by the same scheme, i.e. with hybrid schemes, of which IMEX schemes are a subclass. Nevertheless, for such schemes the method may still work, for example, when central space discretization is applied to first order terms.

The principle of the method is applicable to general initial-boundary value problems in any number of dimensions, but theorems 3.1-3.5 have been derived for the convection-diffusion equation, with the κ-scheme or the fourth order central scheme used for space discretization of the convection term. To illustrate the use of the method, von Neumann stability conditions are derived for a number of schemes. In most cases, sufficient conditions seem not to have been available before.

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