Applying Quantifier Elimination to Stability Analysis of Difference Schemes

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Stability analysis is an important tool for constructing time-stepping finite difference schemes for partial differential equations. This paper describes how von Neumann stability analysis can be reduced to a quantifier elimination problem over the reals. We report our experience in analysing some difference schemes by using a quantifier elimination package based on the partial cylindrical algebraic decomposition algorithm.

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1. INTRODUCTION

Stability is one of the most important properties of difference schemes used for numerically solving time dependent partial differential equations (PDEs). Its importance is stressed by the Lax–Ritchmyer equivalence theorem which states that under certain natural assumptions a scheme is convergent if and only if it is stable. If the algorithm is not stable, then numerical errors will increase with each time step, the solutions usually begin to oscillate with increasing amplitude and become unusable.

There is a condition for stability called the von Neumann condition that is obtained through a Fourier analysis of the difference scheme. The von Neumann condition is an universally quantified formula including equality and inequality which involve rational functions of the trigonometric functions of the quantified variables and the parameters of the differential equation and the difference scheme.

This condition is quite difficult to analyse, even for simple problems. Von Neumann analysis has not yet been done in a completely symbolic way, although such an analysis can be done using symbolic–numeric methods.

This paper first shows how to convert the von Neumann stability condition to a real polynomial quantifier elimination problem following the ideas presented mainly by Ganzha and Vorozhtsov in [19, 6, 5, 14, 7, 8] where different symbolic–numeric approaches for stability analysis have been described.

However, in principle, the von Neumann condition can be solved completely symbolically by quantifier elimination algorithms, for example, by using the cylindrical algebraic decomposition algorithm developed by Collins [3]. Unfortunately, the original implementations of this algorithm can only handle small problems. However, the original algorithm has been greatly improved by Hong and Collins [10, 2, 11] so that its present implementation in the QEPCAD package [10] is capable of handling decidedly non-trivial problems.

This paper presents the results of our first experiments on checking the von Neumann stability condition using the QEPCAD package. Several elementary model problems whose stability properties are already known are presented to show that the method can at least handle simple problems. The most complex problems attempted are the MacCormack difference scheme for one equation in two space dimensions and a difference scheme for a system of three equations in one dimension.

To simplify the notation, only first-order constant-coefficient systems of partial-differential equations (PDEs) and only two time-step numerical schemes for such equations are considered. Note that such systems are time and space translation invariant which will also be used to simplify the discussion.

However, the methods described here apply to substantially more general problems. Fourier method can be applied to numerical schemes including more than two time steps, either directly or by transforming such schemes into a two step numerical scheme by introducing additional discrete functions and additional discrete equations. The characteristic polynomial of the scheme is the quantity of interest for this analysis, and this polynomial is essentially an invariant of such changes in the numerical scheme.

Higher-order systems of PDEs can be reduced to first-order systems by introducing more dependent variables. For linear PDEs with variable coefficients the method is applicable locally by replacing the variable coefficients by constants. For non-linear problems the method can be used locally after linearization.

2. STABILITY PROBLEM

The initial-value problem for a system of first-order linear constant-coefficient partial differential equations (PDEs) is given by

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{D}(\mathbf{u}) = 0\,, \quad \mathbf{u}(0,\mathbf{x}) = \mathbf{f}(\mathbf{x})\,, \tag{1}$$

where $\mathbf{u} = \mathbf{u}(t,\mathbf{x})$ is a vector function depending on the time coordinate t and on space coordinates $\mathbf{x}$, $\mathbf{D}$ is a linear spatial differential operator with constant coefficients, that is, a linear combination of spatial derivatives, and $\mathbf{f}$ is a given vector function. Let K be the number of PDEs in (1) and M be the number of spatial dimensions in this problem. The pure initial-value problem is considered here, so (1) is solved on a spatial region $\Omega = R^M$ for time $t \in (0,T)$. The following vector and multi-index notation will be used:

$$\begin{aligned}
\mathbf{x} &= (x_1, x_2, \cdots x_M)\,;\\
\mathbf{u} &= (u_1, u_2, \cdots u_K)\,;\\
|\mathbf{u}|^2 &= \sum_{1\le k\le K} |u_k|^2\,;\\
\mathbf{j} &= (j_1, j_2, \cdots j_M)\,;\\
\mathbf{j}\cdot\mathbf{m} &= \sum_{1\le p\le M} j_p\, m_p\,;\\
|\mathbf{j}| &= \max_{1\le p\le M} |j_p|\,;\\
\mathbf{j}\mathbf{x} &= (j_1\, x_1, \cdots, j_M\, x_M)\,.
\end{aligned}$$

The Fourier analysis requires a uniform grid, so let $h_t > 0$ be the time step and $\mathbf{h} = (h_1, \cdots, h_M)$ with $h_j > 0$, be the space steps. Now the discrete set of points in space–time is given by

$$\mathbf{x_j} = \mathbf{j}\,\mathbf{h}\,, \quad t_n = n\,h_t\,,$$

and the continuous function $\mathbf{u}$ is approximated by the grid function $\mathbf{u}^n_{\mathbf{j}}$,

$$\mathbf{u}^n_{\mathbf{j}} \approx \mathbf{u}(t_n, \mathbf{x_j})\,.$$

The L^2 norm of the grid function $\mathbf{u}^n$ is defined by

$$||\mathbf{u}^n||^2 = h \sum_{\mathbf{j}} |\mathbf{u}^n_{\mathbf{j}}|^2\,,$$

where $h = h_1\, h_2 \cdots h_M$.

A linear two-step numerical scheme of width N (finite) for the PDEs (1) at the point $(t_n, \mathbf{x_j})$ can be written in the form

$$\begin{aligned}
\sum_{|\mathbf{m}|\le N} \mathbf{A}^1_{\mathbf{m}}\, \mathbf{u}^{n+1}_{\mathbf{j+m}} \;+\; \sum_{|\mathbf{m}|\le N} \mathbf{A}^0_{\mathbf{m}}\, \mathbf{u}^n_{\mathbf{j+m}} &= 0\,,\\
\mathbf{u}^0_{\mathbf{j}} &= \mathbf{v_j}\,,
\end{aligned} \tag{2}$$

where the $\mathbf{v_j}$ are given and the $A^1_{\mathbf{m}}$ and $A^0_{\mathbf{m}}$ are $K \times K$ constant matrices whose entries depend on the parameters of the PDE and the numerical scheme.

A numerical solution of (1) is obtained by solving of the discrete equations (2). However, a numerical solution gives only approximate values of the solution of the PDEs at the grid points. Any numerical solution has some error and, of course, a good numerical solution has an error which is small in some sense. A very important property of a numerical scheme is: How are the errors propagated as the calculation proceeds from time step to time step? When the numerical error of the solution increases with increasing time, the solution may begin to oscillate with larger and larger amplitudes, and consequently be unusable. Intuitively, a numerical algorithm is stable when the numerical errors are not amplified with increasing time. More precisely, stability requires that for $0 \le n\,h_t \le T$, there exist a constant C_T such that for each n

$$||\mathbf{u}^{n+1}_{\mathbf{j}}|| \le C_T\, ||\mathbf{u}^n_{\mathbf{j}}||\,. \tag{3}$$

Here C_T is independent of the step sizes and n but may depend on any other parameters in the PDE or the discretization scheme. Because of the time-translation invariance, condition (3) only need be required for $n = 0$. Note that the stability is purely the property of the difference scheme (2) and has nothing to do with the original initial-value problem (1).

3. REDUCTION TO QUANTIFIER ELIMINATION PROBLEM

This section provides description of the steps which are taken in applying Fourier analysis to the scheme (2) and in transforming the von Neumann stability condition to a quantifier elimination problem over the real field.

3.1. Fourier Transformation

Using the Fourier method the substitution

$$\mathbf{u}^n_{\mathbf{j}} = \mathbf{w}^n e^{i\,\mathbf{k}\cdot\mathbf{x_j}}\,, \tag{4}$$

where $i^2 = -1$, $\mathbf{w}^n$ is a fixed vector and $\mathbf{k} \in R^M$ is a vector of wave numbers, is applied to the difference scheme (2) resulting, after dividing by the exponential on the right-hand side of (4) and setting $n = 0$, in the equation

$$\hat{\mathbf{A}}_1 \mathbf{w}^1 + \hat{\mathbf{A}}_0 \mathbf{w}^0 = 0\,, \tag{5}$$

where the matrices $\hat{\mathbf{A}}_1$ and $\hat{\mathbf{A}}_0$ are given by

$$\hat{\mathbf{A}}_j = \sum_{|\mathbf{m}|\le N} \mathbf{A}^j_{\mathbf{m}}\, e^{i\,\mathbf{k}\cdot\mathbf{x_m}}\,, \quad j = 1,0. \tag{6}$$

We assume that $\hat{\mathbf{A}}_1$ is invertible, which is not a significant restriction, and from (5) we get

$$\mathbf{w}^1 = \mathbf{G}\mathbf{w}^0\,, \tag{7}$$

where the matrix $\mathbf{G}$ is given by

$$\mathbf{G} = -(\hat{\mathbf{A}}_1)^{-1}\hat{\mathbf{A}}_0\,. \tag{8}$$

The matrix $\mathbf{G}$ is the amplification matrix of the numerical scheme (2). It depends on the parameters of the PDE, the discretization, and the Fourier parameters. The wave numbers and the step sizes play the most important role, so $\mathbf{G}$ is written as $\mathbf{G}\,(\mathbf{k}, h_t, \mathbf{h})$.

3.2. The von Neumann Condition

The von Neumann stability condition [17] for solutions which do not grow exponentially, which is the case assumed here, requires that the spectral radius of the amplification matrix (8) be less than or equal to 1 for all values of the wave numbers **k**. The characteristic polynomial for the numerical scheme (2) is the characteristic polynomial of the the amplification matrix **G** and is given by

$$P(\lambda) = \det(\lambda \mathbf{E} - \mathbf{G}) , \qquad (9)$$

where **E** is the unit matrix. The eigenvalues $\lambda_p(\mathbf{k}, h_t, \mathbf{h})$, $1 \le p \le K$, of the amplification matrix (8) are roots of the characteristic polynomial (9). So the stability condition can be expressed as

$$\forall\, \mathbf{k} \in R^M \quad P(\lambda_p(\mathbf{k})) = 0 , \quad |\lambda_p(\mathbf{k})| \le 1 , \quad p = 1, \cdots, K . \qquad (10)$$

Generally this stability condition is only necessary. It is sufficient, for example, in the case of one equation ($K = 1$). Verifying the sufficient condition is usually an even more complicated problem. In any case, the necessary condition for stability gives substantial insight into the stability properties for the difference scheme.

3.3. Initial Transformations

The transformations of the characteristic polynomial (9) performed in this step include:

1. Various simple rational expressions in the parameters of the PDEs and the numerical scheme are replaced by a single symbol, for example, by introducing the CFL (Courant–Friedrichs–Lewy) number, in order to minimize the number of variables appearing in the polynomial. Here, all parameters are real parameters.
2. The exponentials are replaced by trigonometric functions for each space component p:

$$e^{i\, j_p\, \omega_p} = \left(e^{i\, \omega_p}\right)^{j_p} = (\cos(\omega_p) + i \sin(\omega_p))^{j_p} , \qquad (11)$$

   where $\omega_p = k_p\, h_p$.
3. For every p the substitutions $C_p = \cos(\omega_p)$ and $S_p = \sin(\omega_p)$ eliminate all of the trigonometric functions. The universally quantified variables k_p only appear in the arguments of the trigonometric functions, so the original quantifier $\forall k_p \in R$ in (10) can be replaced by the constraint $S_p^2 + C_p^2 = 1$ and quantifiers $\forall S_p \in [-1, 1]$, and $\forall C_p \in [-1, 1]$. For efficiency reasons it is better to have only one quantified variable for every space dimension p, so one of the following eliminations is usually used:
   (a) If possible, eliminate one of the C_p or S_p by using the identity $S_p^2 + C_p^2 = 1$.
   (b) If possible, use trigonometric transformations (e.g. to multiple angles) so that in $P(\lambda)$ there remains only one trigonometric function depending on ω_p.
   (c) Use the transformation $T_p = \tan(\omega_p/2)$, which always eliminates the trigonometric functions, but increases the degree of the polynomial. The cases for which $\tan(\omega_p/2)$ is not defined have to be checked separately. The quantifier $\forall T_p \in R$ is used in this case.
4. The polynomial, which has generally rational coefficients, is transformed to a polynomial with the same roots and polynomial coefficients by multiplying it by the least common multiple of the denominators of the coefficients.
5. If the polynomial is of first degree, then its only root λ_1 is trivially calculated and then the required real quantified formula containing $|\lambda_1|^2 \le 1$ is easily constructed.
6. If the polynomial has non-real coefficients then, as in [19], it is replaced by the product of itself by the polynomial with complex conjugate coefficients, which results in a polynomial with real coefficients that depend on real parameters. The new polynomial has roots that are the roots of $P(\lambda)$ and their complex conjugates. Note that $|\lambda_p| = |\bar{\lambda}_p| \le 1$, so the von Neumann stability condition (10) for the new polynomial is equivalent to the von Neumann condition for $P(\lambda)$.

The characteristic polynomial, (9) after these transformations, is denoted by $\hat{P}(\lambda)$. Now the von Neumann stability condition has been transformed to a universally-quantified polynomial logical formula that contains a polynomial in λ with real polynomial coefficients. Actually it is possible, by denoting the real and imaginary part of λ by new real variables, to transform this formula to a quantified formula over real field. However, it is better to use a complex transformation to eliminate λ, which is the only remaining complex variable in the formula. The next subsections are devoted to a method for this elimination. How to produce the best form of the von Neumann stability condition is still a topic of research.

3.4. Conformal Mapping

The conformal map of the unit circle to the left-half plane: $\lambda = (z+1)/(z-1)$ is used, as proposed by Ganzha and Vorozhtsov [19, 6], to transform the von Neumann condition to the Routh–Hurwitz problem, which is the task of deciding if all roots of a polynomial have negative real parts. Note that even for a characteristic polynomial of degree 2 it is better to use this approach than to directly solve the polynomial equation. The map is applied to the polynomial $\hat{P}(\lambda)$ giving

$$Q(z) = (z-1)^k\, \hat{P}\left(\frac{z+1}{z-1}\right) , \qquad (12)$$

where k is the degree of the polynomial $\hat{P}(\lambda)$. All roots λ_j of polynomial $\hat{P}(\lambda)$ lie inside the unit circle $|\lambda_j| < 1$

if and only if all roots z_j of the polynomial $Q(z)$ have negative real part $\mathrm{Re}(z_j) < 0$ [16]. Note that if $\hat{P}(\lambda)$ has the root $\lambda = 1$ then the degree of polynomial $Q(z)$ is equal to $k - m_1$ where m_1 is the multiplicity of the root $\lambda = 1$. However, for this root the von Neumann stability condition (10) holds, so there is nothing to check.

3.5. Routh–Hurwitz Problem

A polynomial all of whose roots have negative real part is called *stable polynomial* or sometimes a Hurwitz polynomial. By the transformation (12), determining if a difference scheme is stable has been changed to a Routh–Hurwitz problem, i.e. verifying that the polynomial (12) is stable. There are several methods for solving the Routh–Hurwitz problems [16, 4, 15, 19, 6, 14, 7, 8]. Some of these methods, which apply to polynomials with real coefficients, are based on computing the minors of the Hurwitz matrix. We denote the real coefficients (actually real expressions) of polynomial (12) by a_j:

$$Q(z) = a_0 z^n + a_1 z^{n-1} + \cdots + a_n . \tag{13}$$

The Hurwitz matrix has rows that contain shifts of the coefficient of the odd and even powers of z:

$$\begin{pmatrix} a_1 & a_3 & a_5 & \cdots\cdots\cdots & & & a_{2n-1} \\ a_0 & a_2 & a_4 & \cdots\cdots\cdots & & & a_{2n-2} \\ 0 & a_1 & a_3 & \cdots\cdots\cdots & & & a_{2n-3} \\ 0 & a_0 & a_2 & \cdots\cdots\cdots & & & a_{2n-4} \\ \cdots & \cdots & \cdots & \cdots\cdots\cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots \; 0 & a_j & a_{j+2} \; \cdots & a_n \end{pmatrix}$$

where $j = 0$ for even n, $j = 1$ for odd n and $a_k = 0$ for $k > n$. The principal minors of the Hurwitz matrix

$$D_1 = a_1, \quad D_2 = \det \begin{pmatrix} a_1 & a_3 \\ a_0 & a_2 \end{pmatrix},$$

$$D_3 = \det \begin{pmatrix} a_1 & a_3 & a_5 \\ a_0 & a_2 & a_4 \\ 0 & a_1 & a_3 \end{pmatrix}, \quad \cdots$$

are called Hurwitz determinants. The polynomial (13) with $a_0 > 0$ is stable if and only if [4]

$$a_k > 0, \quad D_k > 0, \quad k = 1, \cdots, n .$$

However the sufficient conditions for the polynomial to be stable can be more simply expressed by the Liénard–Chipart stability criteria [4] which state that the polynomial (13) with $a_0 > 0$ is stable if and only if any of the four statements

$$\begin{aligned} & a_0 > 0 \wedge a_n > 0 \wedge a_{n-2} > 0 \wedge a_{n-4} > 0 \wedge \cdots \\ & \quad \wedge D_1 > 0 \wedge D_3 > 0 \wedge \cdots \\ & a_0 > 0 \wedge a_n > 0 \wedge a_{n-2} > 0 \wedge a_{n-4} > 0 \wedge \cdots \\ & \quad \wedge D_2 > 0 \wedge D_4 > 0 \wedge \cdots \\ & a_0 > 0 \wedge a_n > 0 \wedge a_{n-1} > 0 \wedge a_{n-3} > 0 \wedge \cdots \\ & \quad \wedge D_1 > 0 \wedge D_3 > 0 \wedge \cdots \\ & a_0 > 0 \wedge a_n > 0 \wedge a_{n-1} > 0 \wedge a_{n-3} > 0 \wedge \cdots \\ & \quad \wedge D_2 > 0 \wedge D_4 > 0 \wedge \cdots \end{aligned} \tag{14}$$

holds. From these criteria, the simplest can be chosen for a particular problem. Checking that the last Hurwitz determinant satisfies $D_n > 0$ usually requires analysing the most complicated formulas. This can be avoided by using the Liénard–Chipart stability criteria. As the von Neumann stability condition (10) includes the equality $|\lambda_j| = 1$ for the roots λ_j of (9) which corresponds to the equality $\mathrm{Re}(z_j) = 0$ for the roots z_j of (12) we will replace $>$ by $\geq$ in (14).

Now the von Neumann condition (10) has been transformed into the set of inequalities (14) connected by logical operators. These inequalities are universally quantified over the variables resulting from trigonometric functions (usually S_p, C_p or T_p variables). Quantifier elimination by the cylindrical algebraic decomposition algorithm [3, 10, 2, 11] can be used to eliminate the universally quantified variables from this problem. The result is a set of quantifier free inequalities which include the parameters of the difference scheme but not the wave numbers. This is exactly what is needed to understand the stability of the difference scheme.

All steps of this procedure are algorithmic and can be carried out in a computer algebra system.

4. SOFTWARE TOOLS

To verify the applicability of the outlined approach for stability analysis of difference schemes by quantifier elimination the package FIDE [12] realized in the REDUCE [9] computer algebra system and quantifier elimination by the partial cylindrical algebraic decomposition package QEPCAD [10] realized in the SACLIB [1] computer algebra system have been used.

The FIDE package performs the first steps of the method, i.e. calculation of the amplification matrix and characteristic polynomial, transforming the von Neumann condition to a Routh–Hurwitz problem and applying the Liénard–Chipart criteria (14).

The system of inequalities, which is the output of the FIDE package, is the input to the QEPCAD package. The QEPCAD package performs all the tasks necessary for quantifier elimination and returns the quantifier free formulas, the desired stability conditions. The interface between the two packages is not automatic and requires human interaction.

5. EXAMPLES

In this section, several examples are provided that demonstrate how the method for stability analysis of difference schemes, which is described in previous sections, works in practice.

EXAMPLE 5.1. As the first example consider the following family of difference schemes [18] with parameter $a \in [0,1]$,

$$\begin{aligned} &\tfrac{1}{h_t^2}(u_j^{n+1} - 2\,u_j^n + u_j^{n-1}) = \\ &\tfrac{c^2}{h_x^2}\left[a\,(u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1})\right. \\ &\quad +(1-2\,a)\,(u_{j+1}^n - 2u_j^n + u_{j-1}^n) \\ &\quad \left.+\,a\,(u_{j+1}^{n-1} - 2u_j^{n-1} + u_{j-1}^{n-1})\right], \end{aligned} \tag{15}$$

which approximate the one dimensional wave equation

$$\frac{\partial^2 u}{\partial t^2} = c^2\,\frac{\partial^2 u}{\partial x^2}.$$

To transform the difference scheme (15) into a two-step scheme, the variable $v_j^{n+1} = u_j^n$ is introduced. Then the difference scheme to be analysed, which is equivalent to (15), contains two difference equations.

The amplification matrix (8) of this scheme, resulting from the Fourier transformation, is

$$\begin{pmatrix} \frac{2\,(2\,\cos(k_x\,h_x)\,a\,C - \cos(k_x\,h_x)\,C - 2\,a\,C + C - 1)}{2\,\cos(k_x\,h_x)\,a\,C - 2\,a\,C - 1} & -1 \\ 1 & 0 \end{pmatrix},$$

where $C = c^2\,h_t^2/h_x^2 > 0$. The characteristic polynomial (9) of the scheme is

$$\begin{aligned} P(\lambda) = {} & \lambda^2 + 2\,\lambda\,(-2\cos(k_x\,h_x)\,a\,C + \cos(k_x\,h_x)\,C \\ & + 2\,a\,C - C + 1)/(2\cos(k_x\,h_x)\,a\,C\ - 2\,a\,C - 1) + 1. \end{aligned}$$

The polynomial (12), transformed by the conformal mapping, is

$$\begin{aligned} Q(z) &= z^2\,C\,(C_x - 1) + 4\,C_x\,a\,C - C_x\,C - 4\,a\,C \\ &\quad + C - 2 = a_0 z^2 + a_2, \end{aligned}$$

where $C_x = \cos(k_x\,h_x)$. The Routh–Hurwitz problem for this polynomial is to be investigated. Because this polynomial has degree two and one zero coefficient, the Liénard–Chipart criterion (14) is $(a_0 \geq 0 \wedge a_2 \geq 0) \vee (a_0 \leq 0 \wedge a_2 \leq 0)$ which is equivalent to $a_0 a_2 \geq 0$ and gives the quantified formula

$$\begin{aligned} &\forall C_x \in [-1,1], \\ &C(C_x - 1)(4\,C_x\,a\,C - C_x\,C - 4\,a\,C + C - 2) \geq 0, \end{aligned} \tag{16}$$

which is equivalent to the von Neumann stability condition (10) for the scheme (15). So far all of the algebraic calculations have been performed by the FIDE package. The formulas presented above are generated by computer so they are typically not written in the simplest human-style form.

Using the QEPCAD package, the universal quantifier is removed from the formula (16) resulting in the final stability condition of the difference scheme (15):

$$4\,a\,C - C + 1 \geq 0, \quad \text{i.e.} \quad a \geq \frac{1}{4}\left(1 - \frac{h_x^2}{c^2\,h_t^2}\right).$$

Of course this example is very simple and C_x can be eliminated from (16) quite easily manually. However, the example demonstrates all the steps of the method. The next examples require non-trivial quantifier elimination.

EXAMPLE 5.2. Here the first MacCormack difference scheme [13] in the form

$$\begin{aligned} u_{ij}^{n+1} &= \frac{1}{2}\left[u_{ij}^n + \hat{u}_{ij}^n + \frac{a\,h_t}{h_x}(\hat{u}_{i+1,j}^n - \hat{u}_{ij}^n)\right. \\ &\qquad \left. + \frac{b\,h_t}{h_y}(\hat{u}_{i,j+1}^n - \hat{u}_{ij}^n)\right], \\ \hat{u}_{ij}^n &= u_{ij}^n + \frac{a\,h_t}{h_x}(u_{ij}^n - u_{i-1,j}^n) \\ &\qquad + \frac{b\,h_t}{h_y}(u_{ij}^n - u_{i,j-1}^n), \end{aligned} \tag{17}$$

for the 2D advection equation

$$\frac{\partial u}{\partial t} = a\,\frac{\partial u}{\partial x} + b\,\frac{\partial u}{\partial y}.$$

is considered. Note that the variable $\hat{u}_{ij}^n$ can be eliminated from the scheme, producing a standard two-step scheme.

The characteristic polynomial (9) of the scheme (17) is

$$\begin{aligned} P(\lambda) &= \lambda - [1 \\ &+ \; A\,B\,(-\sin(k_x\,h_x)\,\sin(k_y\,h_y) \\ &\qquad - \cos(k_x\,h_x)\cos(k_y\,h_y) \\ &\qquad + \cos(k_x\,h_x) + \cos(k_y\,h_y) - 1) \\ &+ \; A^2\,(\cos(k_x\,h_x) - 1) + B^2\,(\cos(k_y\,h_y) - 1) \\ &+ \; i\,(A\,\sin(k_x\,h_x) + B\sin(k_y\,h_y))] \end{aligned}$$

where $A = a\,h_t/h_x$, $B = b\,h_t/h_y$.

As pointed out in subsection 3.3, item 5, the root λ_1 of $P(\lambda_1) = 0$ is evaluated and the von Neumann condition (10), which has the form $|\lambda_1|^2 \leq 1$, directly gives the quantified formula

$$\begin{aligned} &\forall T_x \in R, \forall T_y \in R, \\ &[A^2\,T_x^2\,(T_y^2 + 1) + 2\,A\,B\,T_x\,T_y\,(T_x\,T_y + 1) \\ &\quad - A\,T_x^2\,(T_y^2 + 1) + B^2\,T_y^2\,(T_x^2 + 1) \\ &\quad - B\,T_y^2\,(T_x^2 + 1)] \\ &[A^2\,T_x^2\,(T_y^2 + 1) + 2\,A\,B\,T_x\,T_y\,(T_x\,T_y + 1) \\ &\quad + A\,T_x^2\,(T_y^2 + 1) + B^2\,T_y^2\,(T_x^2 + 1) \\ &\quad + B\,T_y^2\,(T_x^2 + 1)] \leq 0, \end{aligned} \tag{18}$$

where $T_x = \tan(k_x\,h_x/2)$, $T_y = \tan(k_y\,h_y/2)$. Note that transforming the trigonometric functions into tangents of half angles allows the factorization of the real polynomial $|\lambda_1|^2 - 1$. This factorization greatly simplifies the quantifier elimination task. However, as already mentioned, using the tangents requires checking the special cases in which tangents are not defined. These special cases produce several other quantified formulas, which all together after quantifier elimination, result in the condition

$$|A + B| \leq 1 \wedge |A - B| \leq 1. \tag{19}$$

The calculated quantifier free formula equivalent to (18) in which (19) is included is

$$[(A \geq 0 \wedge B \geq 0) \vee (A \leq 0 \wedge B \leq 0)] \wedge |A + B| \leq 1.$$

Thus the stability condition of the scheme (17) is

$$[(a \geq 0 \wedge b \geq 0) \vee (a \leq 0 \wedge b \leq 0)] \wedge h_t \left| \frac{a}{h_x} + \frac{b}{h_y} \right| \leq 1 .$$

EXAMPLE 5.3. In this example, the system of difference equations [17]

$$\begin{aligned}
\frac{u_j^{n+1} - u_j^n}{h_t} &= c\,\frac{w_{j+1/2}^n - w_{j-1/2}^n}{h_x} \\
&\quad -(\gamma - 1)\frac{e_{j+1/2}^n - e_{j-1/2}^n}{h_x}, \\
\frac{w_{j+1/2}^{n+1} - w_{j+1/2}^n}{h_t} &= c\,\frac{u_{j+1}^{n+1} - u_j^{n+1}}{h_x}, \qquad (20)\\
\frac{e_{j+1/2}^{n+1} - e_{j+1/2}^n}{h_t} &= \sigma\,\frac{e_{j+3/2}^{n+1} - 2e_{j+1/2}^{n+1} + e_{j-1/2}^{n+1}}{h_x^2} \\
&\quad -c\,\frac{u_{j+1}^{n+1} - u_j^{n+1}}{h_x},
\end{aligned}$$

with $c > 0$, $\sigma > 0$, approximating the system of partial differential equations for coupled sound and heat flow

$$\begin{aligned}
\frac{\partial u}{\partial t} &= c\,\frac{\partial\,(w - (\gamma - 1)e)}{\partial x}, \\
\frac{\partial w}{\partial t} &= c\,\frac{\partial u}{\partial x}, \\
\frac{\partial e}{\partial t} &= \sigma\,\frac{\partial^2 e}{\partial x^2} - c\,\frac{\partial u}{\partial x},
\end{aligned}$$

is investigated.

Again the amplification matrix of the difference scheme (20) and its characteristic polynomial $P(\lambda)$ (9) are calculated giving

$$\begin{aligned}
P(\lambda) &= [\lambda^3\,(-4\mu C_x + 4\mu + 1) \\
&+ \lambda^2\,(-4\gamma\nu^2 C_x + 4\gamma\nu^2 + 16\nu^2\mu C_x^2 \\
&\quad -32\nu^2\mu C_x + 16\nu^2\mu + 8\mu C_x - 8\mu - 3) \\
&+ \lambda\,(4\gamma\nu^2 C_x - 4\gamma\nu^2 - 4\mu C_x + 4\mu + 3) \\
&- 1]/(4\mu C_x - 4\mu - 1),
\end{aligned}$$

where $\mu = \sigma h_t/h_x^2$, $\nu = c h_t/h_x$, $C_x = \cos^2(k_x h_x/2)$. This polynomial is transformed, by the conformal mapping, to the polynomial (12) to which the Liénard–Chipart criteria (14) are applied. The calculated inequalities are (using the first line of (14));

$$\begin{aligned}
a_0 &= 16\nu^2\mu\,(C_x^2 - 2C_x + 1) \geq 0; \\
a_1 &= D_1 = 8\nu^2\,(-\gamma C_x + \gamma + 2\mu C_x^2 \\
&\quad -4\mu C_x + 2\mu) \geq 0; \qquad (21)\\
a_3 &= 8\,(\gamma\nu^2 C_x - \gamma\nu^2 - 2\nu^2\mu C_x^2 + 4\nu^2\mu C_x \\
&\quad -2\nu^2\mu - 2\mu C_x + 2\mu + 1) \geq 0; \\
D_3 &= 128\nu^2\mu\,(\gamma C_x^2 - 2\gamma C_x + \gamma - C_x^2 \\
&\quad +2C_x - 1) \geq 0;
\end{aligned}$$

where the quantifier applied to these inequalities is $\forall C_x \in [0,1]$. The quantifier elimination of (21) results in the stability condition of (20):

$$2\mu\nu^2 + \gamma\nu^2 - 2\mu - 1 \leq 0, \qquad \text{i.e.} \quad \nu \leq \sqrt{\frac{1 + 2\mu}{\gamma + 2\mu}},$$

Quantifier elimination problem	*CPU time* [s]
Example 1, (16)	1
Example 2, (18) including (19)	194
Example 2, (18) without (19)	2891
Example 3, (21)	10

TABLE 1. Time requirements for quantifier elimination (DEC 5000/25 with 4 MB of heap memory)

which is the condition presented in [17].

6. DISCUSSION

The bottleneck in the analysis of stability is the extremely high complexity of the quantifier elimination by the cylindrical algebraic decomposition algorithm. Our limited experience with the QEPCAD package shows that either the quantifier elimination problem is solved rather quickly (usually less than a few minutes on a DECstation 5000/25 or PC 486/33) or the solution is not completed at all (not in a few hours of CPU time). Probably the complexity curve is extremely steep quite early. In fact, the complexity of the algorithm is double exponential in number of variables appearing in a quantified formula and polynomial in the total degree of polynomial in the formula.

This complexity estimate and our experience indicates that the number of trigonometric functions appearing in the inequalities (14) which are related to any one coordinate should be minimized, preferably to one function as described in subsection 3.3, item 3. Of course any other substitutions decreasing the number of variables in the formula simplifies the quantifier elimination task. In some cases (see example 2) the polynomial in the inequality can be factorized to produce a simpler quantified formula.

The time requirements for the first part of the method up to the formulation of a quantifier elimination problem are not high. To give an insight into the time requirements of the quantifier elimination task we present here Table 1 which summarizes the time taken by the QEPCAD package for quantifier elimination in examples presented in this paper. The quantifier elimination problem (18) without the conditions (19), which are obtained from the special cases, demonstrates the importance of including all available restriction on non-quantified variables in the quantified formula. The calculations of the conditions (19) requires several runs of QEPCAD. Each run took only several seconds since the number of variables for the special cases is less than the number of variables in the quantified formula (18).

Clearly, further research is needed to find better ways of transforming the von Neumann condition to a quantified formula and doing the quantifier elimination. Hopefully, we will have further insights as we tackle further examples.

7. CONCLUSION

A practical method for stability analysis of difference schemes that uses quantifier elimination by cylindrical algebraic decomposition has been presented. The full algorithm can be implemented in a computer algebra system and is capable of producing an analytic formula for the stability condition of the difference scheme being analysed. The examples section presents the results of some of our first experiments with this method. Several simple examples show the applicability of the method. However, we have to point out that, at present, the method is not usable for very complicated difference schemes mainly because of extremely large computational time and storage requirements for quantifier elimination by the cylindrical algebraic decomposition algorithm. In any case, it is reasonable to hope that the algorithm can be improved sufficiently so that it can be used for analysis of schemes whose stability condition is not yet known.

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