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Quantifier elimination supported proofs in the numerical treatment of fluid flows

Richard Liska · Pavel Váchal

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Abstract During the analysis of numerical methods for fluid flows some properties of numerical methods as stability or monotonicity can be stated as quantified problems and proved by quantifier elimination. A case study demonstrating such proofs is presented. The study shows that the stability region of the central scheme for advection-diffusion equation with Runge–Kutta time discretization is much bigger than classical stability region.

Keywords Quantifier elimination · Stability · Finite difference method

1 Introduction

Fluid flows are typically numerically modeled by finite difference, finite volume or finite element methods. Properties of these numerical methods which are essential for their correct numerical performance include stability, order of approximation, conservation and monotonicity. Analysis of these properties is a crucial part of their design. During the analysis many subproblems can be formulated as quantifier elimination (QE) problems and proved by quantifier elimination methods. A case study demonstrate the usefulness of this approach.

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R. Liska (✉) · P. Váchal
Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague,
Brehova 7, 115 19 Prague 1, Czech Republic
e-mail: liska@siduri.fjfi.cvut.cz

P. Váchal
e-mail: vachal@galileo.fjfi.cvut.cz

The case study originates from incompressible fluid flow Navier–Stokes modeling of atmospheric boundary layer. It deals with the stability analysis of simplified central scheme for the advection-diffusion equation in 1D with Runge–Kutta time discretization. We prove that the real stability domain of the scheme is much bigger than the classical Swanson–Turkel stability limit [13]. Here the originally unsolvable QE problem is transformed by a few tricks into several other solvable QE problems. The contribution of this paper is two-fold. First the proved bigger stability region allows to use bigger time steps in numerical computation, and second the method used to transform the unsolvable QE problem to several simpler ones can be applied to treatment of other difficult QE problems. The stability of finite difference schemes was analyzed by QE methods in [7].

2 Stability of a finite difference scheme

The atmospheric boundary layer is modeled by incompressible Navier–Stokes equations in 3D by the artificial compressibility method [10]

$$\begin{aligned}
\frac{1}{c_s^2} p_t + u_x + v_y + w_z &= 0 \\
u_t + (uu)_x + (uv)_y + (uw)_z &= -\frac{1}{\rho} p_x + (K u_x)_x + (K u_y)_y + (K u_z)_z \\
v_t + (vu)_x + (vv)_y + (vw)_z &= -\frac{1}{\rho} p_y + (K v_x)_x + (K v_y)_y + (K v_z)_z \\
w_t + (wu)_x + (wv)_y + (ww)_z &= -\frac{1}{\rho} p_z + (K w_x)_x + (K w_y)_y + (K w_z)_z
\end{aligned}$$

where ρ is density, p is pressure, u, v, w are three components of velocity, c_s is the artificial sound speed, K is the turbulent diffusion coefficient. The analysis of the numerical method for solving this full 3D non-linear system is currently impossible.

The analysis is performed for the simple linear 1D advection diffusion equation for $u(t, x)$

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = b\frac{\partial^2 u}{\partial x^2}$$

with positive diffusion coefficient $b > 0$. Choosing central differences in space results in a semi-discrete problem for spatial discretization $u_j(t) \approx u(t, j\Delta x)$

$$\frac{d\, u_j}{d\, t} = -a\frac{u_{j+1} - u_{j-1}}{2\Delta x} + b\frac{u_{j+1} - 2u_j + u_{j-1}}{\Delta x^2}.$$

The semi-discrete problem, i.e. the system of ordinary differential equations

$$\frac{d\, U}{d\, t} = L(U)$$

is treated by the second order Runge–Kutta method

$$\begin{aligned}
U^{(0)} &= U^n \\
U^{(1)} &= U^{(0)} + \frac{1}{2}\Delta t L\left(U^{(0)}\right) \\
U^{(2)} &= U^{(0)} + \frac{1}{2}\Delta t L\left(U^{(1)}\right) \\
U^{(3)} &= U^{(0)} + \Delta t L\left(U^{(2)}\right) \\
U^{n+1} &= U^{(3)}
\end{aligned}$$

Introducing numbers $\sigma = \frac{a\Delta t}{\Delta x}, \beta = \frac{b\Delta t}{\Delta x^2} > 0$ the full central finite difference scheme with Runge–Kutta time discretization is defined by the sequence

$$\begin{aligned}
u_j^{(0)} &= u_j^n \\
u_j^{(1)} &= u_j^{(0)} - \frac{\sigma}{4}\left(u_{j+1}^{(0)} - u_{j-1}^{(0)}\right) + \frac{\beta}{2}\left(u_{j+1}^{(0)} - 2u_j^{(0)} + u_{j-1}^{(0)}\right) \\
u_j^{(2)} &= u_j^{(0)} - \frac{\sigma}{4}\left(u_{j+1}^{(1)} - u_{j-1}^{(1)}\right) + \frac{\beta}{2}\left(u_{j+1}^{(1)} - 2u_j^{(1)} + u_{j-1}^{(1)}\right) \qquad (1) \\
u_j^{(3)} &= u_j^{(0)} - \frac{\sigma}{2}\left(u_{j+1}^{(2)} - u_{j-1}^{(2)}\right) + \beta\left(u_{j+1}^{(2)} - 2u_j^{(2)} + u_{j-1}^{(2)}\right) \\
u_j^{n+1} &= u_j^{(3)}.
\end{aligned}$$

The stability analysis of the central scheme (1) is performed by the standard Fourier method [11] by performing the transformation $u_{j+J} \rightarrow \hat{u}e^{iJ\xi}$ introducing the discrete Fourier transformation $\hat{u}$ in the space of the discrete grid function u_j. The amplification factor $g(\xi, \sigma, \beta)$ is defined by substituting $u_j^{(0)}, u_j^{(1)}, u_j^{(2)}, u_j^{(3)}$ from the previous equations into the last equation of (1)

$$\hat{u}^{n+1} = g(\xi, \sigma, \beta)\hat{u}^n.$$

The amplification factor $g(\xi, \sigma, \beta)$ is complex. The von Neumann stability condition [11] then states that the scheme (1) is stable if and only if the norm of the amplification factor is at most one for all Fourier variables ξ, i.e.,

$$\forall \xi, \quad |g(\xi, \sigma, \beta)| \leq 1.$$

This is a QE problem and if we succeed to eliminate the quantifier we would obtain the stability condition of our scheme (1).

We restate the QE problem as

$$\forall y \in [-2, 0], \quad P(y, \sigma, \beta) \leq 0,$$

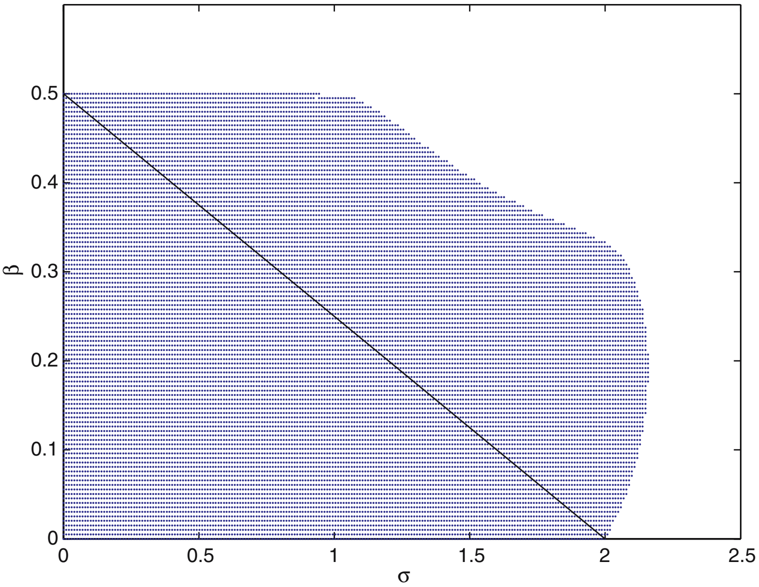

Fig. 1 Approximate stability region of scheme (1) obtained by numerical sampling (the scheme is stable at each plotted point) with Swanson–Turkel stability limit [13] $\beta \le -|\sigma|/4 + 1/2$

where $y = \cos\xi - 1$ and P is a polynomial defined by

$$\frac{1}{16}(1-\cos\xi)P(\cos\xi - 1, \sigma, \beta) = |g(\xi, \sigma, \beta)|^2 - 1$$

So now we have the following QE problem with three variables $\beta, \sigma_2 = \sigma^2, y$

$$\begin{aligned}\forall y \in [-2, 0],\ & \left(48\beta^4\sigma_2 + \sigma_2^3 - 12\beta^2\sigma_2^2 - 64\beta^6\right) y^5 \\ & + \left(-128\beta^5 + 6\sigma_2^3 + 64\beta^3\sigma_2 + 96\beta^4\sigma_2 - 48\beta^2\sigma_2^2 - 8\beta\sigma_2^2\right) y^4 \\ & + \left(32\beta^2\sigma_2 - 192\beta^4 - 32\beta\sigma_2^2 - 48\beta^2\sigma_2^2 + 128\beta^3\sigma_2 + 12\sigma_2^3 + 4\sigma_2^2\right) y^3 \\ & + \left(8\sigma_2^3 - 192\beta^3 + 64\beta^2\sigma_2 - 32\beta\sigma_2^2 + 16\sigma_2^2 - 16\beta\sigma_2\right) y^2 \\ & + \left(-32\beta\sigma_2 + 16\sigma_2^2 - 128\beta^2\right) y - 64\beta \le 0.\end{aligned} \tag{2}$$

This is a difficult QE problem that cannot be solved in reasonable time. The QEPCAD run for this problem failed after 14 h of CPU time (on a 2.6 GHz machine) on *Prime list exhausted* error message with allocated 256 MB of memory and 1,000,000 primes. So we have to use another approach to solve this difficult QE problem.

To get a first estimate of the stability region we have performed numerical sampling over appropriate intervals for the three variables β, σ_2, y and obtained the approximate stability region shown in Fig. 1 together with the classical Swanson–Turkel stability limit [13]. The approximate stability region suggested us to split the solution of the original QE problem (2) into two cases by splitting the 2D (σ, β) space along the line $\sigma = 1$ into regions $\sigma \leq 1$ and $\sigma > 1$. Limiting σ to $\sigma \in [0, 1]$ in QE problem (2), QEPCAD quickly found (in 2 s of CPU time on 2.6 GHz machine) that it is equivalent to $\beta \leq 1/2$. This is the stability condition for $\sigma \in [0, 1]$.

The second case for $\sigma > 1$ is more complicated. When we look at the projection factors of the QE problem (2), we find that the discriminant of the initial polynomial according to y is

$$\begin{aligned}
D = {} & 786,432\beta^{15} + 4,456,448\sigma_2\beta^{14} + 22,167,552\sigma_2^2\beta^{13} - 4,653,056\sigma_2\beta^{13} \\
& - 19,218,432\sigma_2^3\beta^{12} - 5,750,784\sigma_2^2\beta^{12} + 46,855,168\sigma_2^4\beta^{11} - 15,237,120\sigma_2^3\beta^{11} \\
& + 8,511,488\sigma_2^2\beta^{11} - 22,474,752\sigma_2^5\beta^{10} - 28,515,328\sigma_2^4\beta^{10} + 854,016\sigma_2^3\beta^{10} \\
& + 9,664,512\sigma_2^6\beta^9 + 12,542,976\sigma_2^5\beta^9 + 22,981,888\sigma_2^4\beta^9 - 3,314,688\sigma_2^3\beta^9 \\
& - 1,204,736\sigma_2^7\beta^8 - 9,535,488\sigma_2^6\beta^8 - 8,913,920\sigma_2^5\beta^8 - 7,008,256\sigma_2^4\beta^8 \\
& + 33,792\sigma_2^8\beta^7 + 333,824\sigma_2^7\beta^7 + 7,291,264\sigma_2^6\beta^7 + 3,420,928\sigma_2^5\beta^7 \\
& + 1,500,160\sigma_2^4\beta^7 - 384\sigma_2^8\beta^6 + 393,088\sigma_2^7\beta^6 - 3,746,432\sigma_2^6\beta^6 \\
& - 1,049,856\sigma_2^5\beta^6 - 2,816\sigma_2^{10}\beta^5 + 16,896\sigma_2^9\beta^5 - 41,984\sigma_2^8\beta^5 - 408,512\sigma_2^7\beta^5 \\
& + 1,347,872\sigma_2^6\beta^5 + 148,352\sigma_2^5\beta^5 + 2,816\sigma_2^{10}\beta^4 - 16,096\sigma_2^9\beta^4 + 33,568\sigma_2^8\beta^4 \\
& + 16,0384\sigma_2^7\beta^4 - 290,880\sigma_2^6\beta^4 - 1,408\sigma_2^{10}\beta^3 + 7,680\sigma_2^9\beta^3 - 12,140\sigma_2^8\beta^3 \\
& - 27,088\sigma_2^7\beta^3 + 26,784\sigma_2^6\beta^3 + 344\sigma_2^{10}\beta^2 - 1,736\sigma_2^9\beta^2 + 1,636\sigma_2^8\beta^2 \\
& + 1,224\sigma_2^7\beta^2 - 24\sigma_2^{10}\beta + 112\sigma_2^9\beta - 27\sigma_2^8\beta + 108\sigma_2^7\beta - 2\sigma_2^{10} + 8\sigma_2^9
\end{aligned}$$

When we plot in Fig. 2 the curve $D = 0$ defined by the discriminant D and compare it with the approximate stability domain in Fig. 1, we see that the shape of the approximate stability domain for $\sigma > 1$ is close to the curve defined by the discriminant. This suggests that the curve $D = 0$ might be the border of the stability domain.

Indeed, QEPCAD proved easily that for $\sigma \geq 1$ the stability condition is $D \geq 0$ (in 5 s CPU time on 2.6 GHz machine). In fact for $\sigma \geq 1$ QEPCAD has proved that two QE problems (giving necessary and sufficient conditions for QE problem (2) for $\sigma \geq 1$) are equivalent to true. The first QE problem for the area inside the stability region is

$$\forall\sigma_2\forall\beta\forall y, \quad (1 \leq \sigma_2 \wedge 0 \leq \beta \leq 1/2 \wedge -2 \leq y \leq 0 \wedge D \geq 0) \Rightarrow P \leq 0,$$

while the second QE problem for area outside the stability region has to be stated as

$$\forall\sigma_2\forall\beta\exists y, (1 \leq \sigma_2 \wedge 0 \leq \beta \wedge (\beta > 1/2 \vee D < 0)) \Rightarrow (-2 \leq y \leq 0 \wedge P > 0) \quad (3)$$

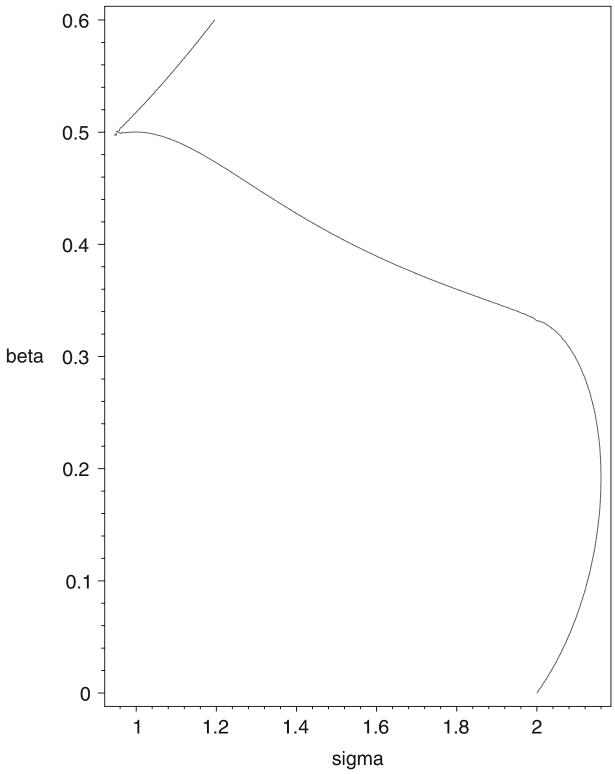

Fig. 2 The curve defined by the discriminant $D = 0$

Note that the usage of Brown's *for all but finitely many* quantifiers from his QEPCAD B [1] allowed to prove that the second QE problem (3) is equivalent to true while the standard *for all* quantifiers resulted again in the *Prime list exhausted* error message. As we are not interested in isolated stability points in σ_2, β plane we can use the *for all but finitely many* quantifiers.

The zoom of the critical part of curve $D = 0$ around the point $\sigma = 1, \beta = 1/2$ presented in Fig. 3 reveals a cusp on the curve at a point given by an algebraic number defined by a high degree polynomial. This is probably the reason for the huge complexity of initial QE problem (2).

To summarize we proved that the stability region of the scheme (1) is much bigger than the classical Swanson–Turkel stability region $\beta \leq -|\sigma|/4 + 1/2$, which can be seen in Fig. 1. The bigger stability region allows to use bigger time step in numerical computation which speeds up the computation and also improves the numerical results.

3 QE tools employed

In this section we summarize the QE tools which we employ in the analysis of numerical methods for fluid flows and review a little bit our experience with these tools. The

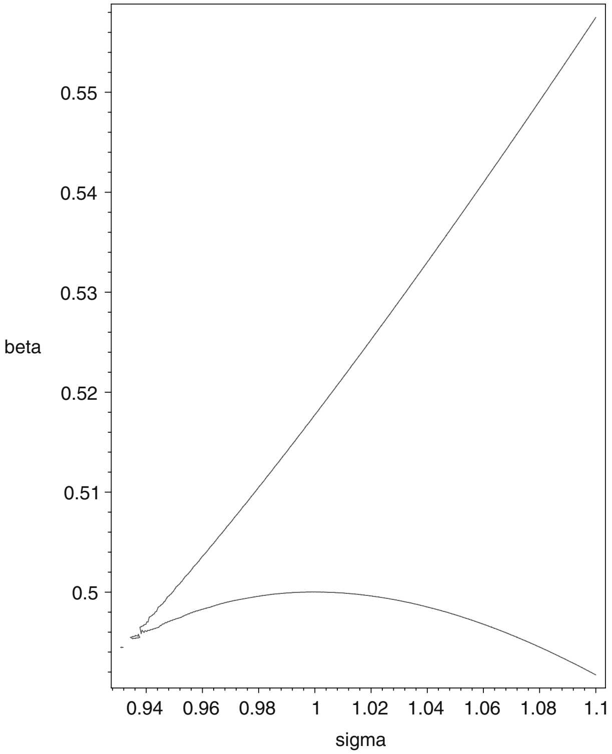

Fig. 3 Zoom of the curve defined by the discriminant $D = 0$ around the point $\sigma = 1$, $\beta = 1/2$

only QE method able to deal with any QE problem over real closed fields is Collins cylindrical algebraic decomposition (CAD) method [3] improved to partial CAD by Collins and Hong [4]. The first and for a long time the only implementation of partial CAD method was Hong's program QEPCAD [6] which we use most often. Recently QEPCAD is maintained by Brown as QEPCAD B [1] with several extensions. For us the most important extension is the new quantifier "for all but finitely many" as in many our QE problems it can be used instead of general standard "for all" quantifier. In general this replacement speeds up the QE process and in some cases as e.g., for QE problem (3) this replacement turns an unsolvable problem to a solvable one. Another useful extension of Brown's is the program SLFQ [2] which uses QEPCAD B for simplifying quantifier free formulas and which often simplifies a lot lengthy results of virtual substitution method in REDLOG.

REDLOG [5] is the second QE package being developed for a long time. It incorporates several QE methods. The virtual substitution method [14] is able to deal with many variables, however it can treat just low degree polynomials. Recently REDLOG also includes implementation of partial CAD method.

In recent years the partial CAD method has been implemented also in Maple [15] and Mathematica [12]. Sometimes we also use the AQCS program [8,9] for approximate QE.

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