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On Stability of Numerical Methods for Systems of Initial-Value Partial Differential Equations

In a previous paper [1], it was demonstrated that difference approximations to the initial-value partial differential equation defined on R: $\{0 \leqslant t \leqslant T, -\infty < x < \infty\}$

$$\frac{\partial^n u}{\partial t^n} = \sum_{i=0}^{n-1} \alpha_i{}' \frac{\partial^i u}{\partial t^i} = \sum_{i=0}^{n-1} \sum_{r=0}^{g} c_{ir} \frac{\partial^r}{\partial x^r} \frac{\partial^i u}{\partial t^i} \tag{1}$$

must satisfy certain "invariant" quantities in order that the difference approximation be numerically stable as the time step approaches zero, $\Delta t \to 0$, for a fixed space step, Δx.

The utility of these results is the "invariant" quantities yield a priori knowledge on the type of difference schemes which should be used to approximate (1) as well as an estimate for Δt. If the "invariants" are satisfied and are nonzero except for space frequencies $k = 0$, $2\pi/\Delta x$, $4\pi/\Delta x$,..., then a stable numerical process is assured for sufficiently small Δt. Stability is defined in the sense of Von Neumann [2] and is shown in [1] to depend predominately on the terms of index $r \geqslant 1$ in equation (1).

Equation (1) may be put into matrix form, and if the c_{ir} are constant coefficients, the "invariant" properties hold under a linear, non-singular transformation of coordinates. To demonstrate this property consider the second order system of linear, constant coefficient, partial differential equations corresponding to $n = 2$ in equation (1):

$$\frac{\partial}{\partial t} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \begin{bmatrix} \alpha_{11}' & \alpha_{12}' \\ \alpha_{21}' & \alpha_{22}' \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} \tag{2}$$

The space derivatives α_{ij}' may be approximated by mesh displacements on $R_D : \{0 \leqslant m\,\Delta t \leqslant T, n\,\Delta x = x\}$ at either the $(m + 1)\,\Delta t$ or $m\,\Delta t$ time steps and the equation Fourier transformed with respect to the space axis to yield a form to establish stability of the numerical scheme:

$$\begin{bmatrix} v_1(t + \Delta t, k) \\ v_2(t + \Delta t, k) \end{bmatrix} = \begin{bmatrix} 1 + \theta_1 \alpha_{11}\,\Delta t & \theta_2 \alpha_{12}\,\Delta t \\ \theta_3 \alpha_{21}\,\Delta t & 1 + \theta_4 \alpha_{22}\,\Delta t \end{bmatrix}^{-1}$$
$$\times \begin{bmatrix} 1 + \Delta t(1 + \theta_1)\,\alpha_{11} & \Delta t(1 + \theta_2)\,\alpha_{12} \\ \Delta t(1 + \theta_3)\,\alpha_{21} & 1 + \Delta t(1 + \theta_4)_{22} \end{bmatrix} \begin{bmatrix} v_1(t, k) \\ v_2(t, k) \end{bmatrix} \tag{3}$$

k is Fourier or dual variable and $\alpha_{ij}v(t, k)$ corresponds to the transform of the difference approximation to $\alpha'_{ij}v(t, x)$ as developed in [*1*]. The θ_i are real but otherwise arbitrary.

The roots of the characteristic polynomial of (3) must satisfy the Von Neumann stability condition [*2*]. When the characteristic polynomial of (3) is introduced into the Schur–Cohn Criterion as done in [*1*], the "lowest power" Δt terms in the expansion of the determinants are found to be independent of the arbitrary θ_i. Thus the "invariants" are:

$$\Delta_1 \cong \Delta t(\alpha_{11} + \bar{\alpha}_{11} + \bar{\alpha}_{22} + \bar{\alpha}_{22}) < 0 \tag{4}$$

$$\begin{aligned}\Delta_2 \cong \Delta t^4(\alpha_{11} + \bar{\alpha}_{11} + \alpha_{22} + \bar{\alpha}_{22})[\alpha_{11}\bar{\alpha}_{11}(\alpha_{22} + \bar{\alpha}_{22}) + \alpha_{22}\bar{\alpha}_{22}(\alpha_{11} + \bar{\alpha}_{11}) \\ - (\alpha_{22}\bar{\alpha}_{12}\bar{\alpha}_{21} + \bar{\alpha}_{22}\alpha_{12}\alpha_{22}) - (\alpha_{11}\bar{\alpha}_{12}\bar{\alpha}_{21} + \bar{\alpha}_{11}\alpha_{12}\alpha_{21})] + (\alpha_{11}\alpha_{22} - \bar{\alpha}_{11}\bar{\alpha}_{22})^2 \\ - 2(\alpha_{11}\alpha_{22} - \bar{\alpha}_{11}\bar{\alpha}_{22})(\alpha_{12}\alpha_{21} - \bar{\alpha}_{12}\bar{\alpha}_{21}) + (\alpha_{12}\alpha_{21} - \bar{\alpha}_{12}\bar{\alpha}_{21})^2 > 0\end{aligned} \tag{5}$$

where the higher order Δt terms are dependent on the θ_i.

Δ_1 must be negative and Δ_2 positive for all k in order that both roots of (3) lie inside the unit circle. It is seen that this can be accomplished if Δt is sufficiently small that the lowest power Δt term (the invariants) dominate Δ_1 and Δ_2 and the α_{ij} have the proper signs for all space frequencies k (e.g. $\alpha = (e^{jk\Delta x} - 1)/\Delta x$ for a first derivative approximation).

The important point is that (2) has the same characteristic equation as:

$$\frac{\partial}{\partial t}\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ \alpha_0' & \alpha_1' \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \tag{6}$$

when $\alpha_1' = \alpha'_{11} + \alpha'_{22}$ and $\alpha_0' = \alpha'_{12}\alpha'_{21} - \alpha'_{11}\alpha'_{22}$. Approximations to (6) have the "invariants" [*1*]:

$$\Delta_1 = \Delta t(\alpha_1 + \bar{\alpha}_1) < 0 \tag{7}$$

$$\Delta_2 = \Delta t^4(\alpha_0 - \bar{\alpha}_0)^2 - \Delta t^4(\alpha_1 + \bar{\alpha}_1)(\alpha_0\bar{\alpha}_1 + \bar{\alpha}_0\alpha_1) > 0 \tag{8}$$

which are the same as (4) and (5) under the substitution. The higher order Δt terms are in general not equal. In [*1*] it was shown that the invariant quantities also appear when a multi-step method (more than three time steps) is used to approximate the second order characteristic equation. Since the "invariants" are fundamental to difference approximations, it is possible to determine apriori if a stable formulation can be found for an equation or system of equations by means of examining the "invariants". Such a classification is presented in Table I for the second order equation. In this table, there are eighty categories which depend on combinations

TABLE I CLASSIFICATION OF A SECOND ORDER SYSTEM

α_0 \ α_1	$\mathrm{Re}\,\alpha_1=0$ $\mathrm{Im}\,\alpha_1=0$	$\mathrm{Re}\,\alpha_1\leq 0$ $\mathrm{Im}\,\alpha_1=0$	$\mathrm{Re}\,\alpha_1\leq 0$ $\mathrm{Im}\,\alpha_1\gtrless 0$	$\mathrm{Re}\,\alpha_1\leq 0$ $\mathrm{Im}\,\alpha_1\lessgtr 0$	$\mathrm{Re}\,\alpha_1=0$ $\mathrm{Im}\,\alpha_1\gtrless 0$	$\mathrm{Re}\,\alpha_1=0$ $\mathrm{Im}\,\alpha_1\lessgtr 0$	$\mathrm{Re}\,\alpha_1\geq 0$ $\mathrm{Im}\,\alpha_1=0$	$\mathrm{Re}\,\alpha_1\geq 0$ $\mathrm{Im}\,\alpha_1\gtrless 0$	$\mathrm{Re}\,\alpha_1\geq 0$ $\mathrm{Im}\,\alpha_1\lessgtr 0$
$\mathrm{Re}\,\alpha_0=0$ $\mathrm{Im}\,\alpha_0=0$		1	2	3	4	5	6 ////// POSSIBLE	7 //////	8 //////
$\mathrm{Re}\,\alpha_0\leq 0$ $\mathrm{Im}\,\alpha_0=0$	9	10 F.N.F.	11 F.N.F.	12 F.N.F.	13	14	15 //////	16 ////// FINAL	17 //////
$\mathrm{Re}\,\alpha_0\leq 0$ $\mathrm{Im}\,\alpha_0\gtrless 0$	18 ══	19 F.N.F.	20 F.N.F.	21	22 ══	23 ══	24 //////	25 ////// VALUE	26 //////
$\mathrm{Re}\,\alpha_0\leq 0$ $\mathrm{Im}\,\alpha_0\lessgtr 0$	27 ══	28 F.N.F.	29	30 F.N.F.	31 ══	32 ══	33 //////	34 ////// PROBLEMS	35 //////
$\mathrm{Re}\,\alpha_0=0$ $\mathrm{Im}\,\alpha_0\gtrless 0$	36 ══	37 ══	38 F.N.F.	39 ══	40 ══	41 ══	42 ══	43 ══	44
$\mathrm{Re}\,\alpha_0=0$ $\mathrm{Im}\,\alpha_0\lessgtr 0$	45 ══	46 ══	47 ══	48 F.N.F.	49 ══	50 ══	51 ══	52	53 ══
$\mathrm{Re}\,\alpha_0\geq 0$ $\mathrm{Im}\,\alpha_0=0$	54 //////	55 ══	56 ══	57 ══	58	59	60 ══	61 ══	62 ══
$\mathrm{Re}\,\alpha_0\geq 0$ $\mathrm{Im}\,\alpha_0\gtrless 0$	63 ══	64 ══	65	66 ══	67 ══	68 ══	69 ══	70 ══	71 //////
$\mathrm{Re}\,\alpha_0\geq 0$ $\mathrm{Im}\,\alpha_0\lessgtr 0$	72 ══	73 ══	74 ══	75	76 ══	77 ══	78 ══	79 //////	80 ══

Notes: [Highest even order of α_1]$^2 \geq$ [odd order α_0], ══ (unstable), Im ( ) $\gtrless$ 0 means $f(k\Delta x)\sin k\Delta x$, with $f(k\Delta x)\geq 0$

of the real and imaginary parts of α_0 and α_1. These categories are divided into four groups. These groups are:

1) F.N.F. which means that any difference expression to (5) or (12) that results in the α_0 and α_1 listed is a stable formulation when Δt is sufficiently small that the invariant quantities dominate the Schur–Cohn determinants.

2) ══ means that the invariants are not the proper sign so that the difference equation is unstable for small Δt. Usually one root will be inside the unit circle and one root outside the unit circle.

3) (blank) means that combinations of θ_i may be chosen such that a stable formulation is found. The wave equation $\partial^2 u/\partial t^2 = \partial^2 u/\partial x^2$ is represented by category #9. Many of the implicit or explicit schemes used for this equation can be considered cases of particular θ_i for (3).

4) ////// means that equation (7) is greater than zero, and both roots of the characteristic equation lie outside the unit circle. In this circumstance, it may be possible to formulate the difference equation as a *final-value problem* and proceed to solve the equation backwards in time. Laplace's equation, $\partial^2 u/\partial t^2 = -\partial^2 u/\partial x^2$, is one example which may be represented by category #54.

Two constraints are noted in Table I. The first is the real part of the coefficient of the Fourier transform for α_i must be definite. That is Re $\alpha_i \geqslant 0$ or Re $\alpha_i \leqslant 0$ for all k in order the "invariants" to be proper sign. Also for the same difference approximation: Im $\alpha_i = \mathrm{Sin}(k\,\Delta x)\, f(k\,\Delta x)$ where $f(k\,\Delta x)$ is definite. It is possible to generate a family of difference expressions for all orders of space derivatives with this property.

The second constraint is on the magnitude of the coefficients and the order of the derivatives. This is seen from equation (8) to be:

$$\begin{bmatrix}\text{highest order } \alpha_1\\ \text{derivative}\end{bmatrix}^2 \geqslant \begin{bmatrix}\text{highest odd order}\\ \alpha_0 \text{ derivative}\end{bmatrix}$$

for the cases where α_1' is not zero, such that (8) is positive.

In principle, these results extend to higher order systems but the algebraic difficulty increases. The third invariant for a third order equation contains nine or 3^2 terms, such that the nth invariant for an nth order equation perhaps may contain $n^{(n-1)}$ terms. Finding the types of higher order types of equations for which a stable difference scheme can be formulated is correspondingly difficult.

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