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VON NEUMANN STABILITY OF THE WONDY WAVECODE FOR THERMODYNAMIC EQUATIONS OF STATE

MASTER

D. L. Hicks

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VON NEUMANN STABILITY OF THE WONDY WAVECODE FOR THERMODYNAMIC EQUATIONS OF STATE

D. L. Hicks
Computational Physics & Mechanics Division I - 5162
Sandia Laboratories, Albuquerque, New Mexico 87115

ABSTRACT

Previous analyses of the von Neumann stability of the WONDY wavecode (based on the von Neumann-Richtmyer artificial viscosity method) assumed a mechanical stress-strain relation; i.e., they assumed the stress p to depend only on the mass density ρ. In a thermodynamic equation of state p is allowed to depend also on the specific entropy S (or on the specific internal energy $\mathcal{E}$). If p does not depend on $\mathcal{E}$ (or S), then the Grüneisen parameter Γ is zero. Herein a von Neumann stability analysis of WONDY is done for the more general case when $\Gamma \neq 0$. The result of this analysis is the requirement that the timestep be less than the product of the material increment and a certain function f of the acoustic impedance (a), artificial viscosity coefficient Λ, and Γ. In a region of compression if $\Lambda\Gamma > 0$, then $f(a,\Lambda,\Gamma)$ is smaller than $f(a,\Lambda,0)$. Therefore, the more general stability analysis yields the result that the timestep restriction now in WONDY may be insufficient for stability in certain regions of certain calculations.

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1. INTRODUCTION

Wavecodes based on the artificial viscosity method of von Neumann-Richtmyer [1] (e.g., CHARTD, PUFF, WONDY, etc.) require timestep restrictions in order to be stable in the sense of von Neumann (see [2]). Previous stability analyses of the von Neumann-Richtmyer method were done by J. von Neumann and R. Richtmyer in 1950 (see [1]), G. N. White in 1954 (see [3], p. 13), and R. J. Thompson in 1966 (see the appendix of [4]). Those stability analyses were done for what essentially amounts to mechanical stress-strain relations. That is, in the course of those analyses, simplifying assumptions were made which essentially amount to assuming that the pressure was dependent only on the mass density. If the pressure does not depend on the specific internal energy, then the Grüneisen parameter is zero. Herein the stability analysis is done for the more general case when the parameter may be nonzero.

Section two gives the notation, nomenclature, and a description of the WONDY difference scheme.

Section three gives some lemmas about quadratic inequalities and stability; these are the main mathematical tools used in section four.

Section four gives the main results about the timestep restrictions required for the von Neumann stability of WONDY.

Section five gives a summary, conclusions, and recommendations about modifying the timestep restrictions in WONDY and CHART D.

2. NOTATION AND NOMENCLATURE

The equation

$$\frac{\partial V}{\partial t} = \frac{\partial u}{\partial \mu} \tag{2.1}$$

expresses the conservation of volume; t is time; μ is material coordinate; V is specific volume; V is the reciprocal of the mass density ρ; and u is specific momentum. The equation

$$\frac{\partial u}{\partial t} = - \frac{\partial \sigma}{\partial \mu} \tag{2.2}$$

expresses the conservation of momentum; σ is the total stress (taken positive in compression); it is composed of a viscous stress q and an inviscid stress p; i.e.,

$$\sigma = p + q \ . \tag{2.3}$$

The conservation of energy law leads to

$$\frac{\partial E}{\partial t} = - \frac{\partial u\sigma}{\partial \mu} \ ; \tag{2.4}$$

E is the specific total energy; it is composed of the specific internal energy $\mathcal{E}$ and the specific kinetic energy $\frac{1}{2} u^2$; i.e.,

$$E = \mathcal{E} + \frac{1}{2} u^2 \ . \tag{2.5}$$

The equation

$$T \frac{\partial S}{\partial t} = \frac{\partial \mathcal{E}}{\partial t} + p \frac{\partial V}{\partial t} \tag{2.6}$$

follows from the chain rule and definitions of p and T; T is the absolute temperature; and S is the specific entropy. From (2.1) - (2.5) it follows that

$$\frac{\partial \mathcal{E}}{\partial t} = -\sigma \frac{\partial V}{\partial t} . \tag{2.7}$$

WONDY differences this equation rather than (2.5). From (2.6) and (2.7) follows

$$T \frac{\partial S}{\partial t} = -q \frac{\partial V}{\partial t} ; \tag{2.8}$$

by the principle of increasing entropy Eqn. (2.8) yields

$$\text{sign}(q) = -\text{sign}\left(\frac{\partial V}{\partial t}\right) . \tag{2.9}$$

Eqn. (2.9) suggests that q is of the form

$$q = -\Lambda \frac{\partial V}{\partial t} ; \tag{2.10}$$

where Λ is nonnegative and Λ is called the coefficient of viscosity. From (2.1) and (2.10) it follows that

$$q = -\Lambda \frac{\partial u}{\partial \mu} . \tag{2.11}$$

The acoustic impedance (a), the Grüneisen parameter Γ, and the absolute temperature T, are defined by:

$$a^2 = -\left.\frac{\partial p}{\partial V}\right|_S ; \tag{2.12}$$

$$\Gamma = V \left.\frac{\partial p}{\partial \mathcal{E}}\right|_V ; \tag{2.13}$$

and

$$T = \left.\frac{\partial \mathcal{E}}{\partial S}\right|_V . \tag{2.14}$$

It follows that

$$\left.\frac{\partial p}{\partial S}\right|_V = \Gamma\rho T \ . \qquad (2.15)$$

From

$$\frac{\partial p}{\partial t} = \left.\frac{\partial p}{\partial V}\right|_S \frac{\partial V}{\partial t} + \left.\frac{\partial p}{\partial S}\right|_V \frac{\partial S}{\partial t}$$

and Eqns. (2.12) - (2.15) follows

$$\frac{\partial p}{\partial t} = -a^2 \frac{\partial V}{\partial t} + \Gamma\rho T \frac{\partial S}{\partial t} \ . \qquad (2.16a)$$

From Eqns. (2.8) and (2.16a) follows

$$\frac{\partial p}{\partial t} = -(a^2 + \Gamma\rho q) \frac{\partial V}{\partial t} \ . \qquad (2.16b)$$

It is conceptually convenient to define the augmented acoustic impedance a^+ by

$$(a^+)^2 = a^2 + \Gamma\rho q \ .$$

[$(a^+)^2$ is also called the instantaneous acoustic impedance.] Then (2.16b) may be written

$$\frac{\partial p}{\partial t} = -(a^+)^2 \frac{\partial V}{\partial t} \ . \qquad (2.16c)$$

From Eqns. (2.3) and (2.16c) it follows that the total stress rate relation is

$$\frac{\partial \sigma}{\partial t} + (a^+)^2 \frac{\partial V}{\partial t} - \frac{\partial q}{\partial t} = 0 \ . \qquad (2.17)$$

(It is interesting to note the relationship of (2.17) to the generalized Maxwell form for relaxing materials.)

Discrete Notation: Let f_j^n be the numerical approximation to $f(t^n,\mu_j)$. The WONDY difference equation for Eqn. (2.2) is given by:

$$\left(\frac{\Delta u}{\Delta t}\right)_j^n = -\left(\frac{\Delta\sigma}{\Delta\mu}\right)_j^n ; \qquad (2.18)$$

where

$$\left(\frac{\Delta u}{\Delta t}\right)_j^n = \frac{u_j^{n+1/2} - u_j^{n-1/2}}{t^{n+1/2} - t^{n-1/2}} ;$$

and

$$\left(\frac{\Delta\sigma}{\Delta\mu}\right)_j^n = \frac{\sigma_{j+1/2}^n - \sigma_{j-1/2}^n}{\mu_{j+1/2} - \mu_{j-1/2}} .$$

The WONDY difference equation for Eqn. (2.1) is given by:

$$\left(\frac{\Delta V}{\Delta t}\right)_{j+1/2}^{n+1/2} = \left(\frac{\Delta u}{\Delta\mu}\right)_{j+1/2}^{n+1/2} ; \qquad (2.19)$$

where

$$\left(\frac{\Delta V}{\Delta t}\right)_{j+1/2}^{n+1/2} = \frac{V_{j+1/2}^{n+1} - V_{j+1/2}^n}{t^{n+1} - t^n} ;$$

and

$$\left(\frac{\Delta u}{\Delta\mu}\right)_{j+1/2}^{n+1/2} = \frac{u_{j+1}^{n+1/2} - u_j^{n+1/2}}{\mu_{j+1} - \mu_j} .$$

The WONDY difference scheme for stress rate relations of the form (2.17) is given by:

$$\left(\frac{\Delta\sigma}{\Delta t}\right)_{j+1/2}^{n+1/2} = -[(a^+)^2]_{j+1/2}^{n+} \left(\frac{\Delta u}{\Delta\mu}\right)_{j+1/2}^{n+1/2} + \left(\frac{\Delta g}{\Delta t}\right)_{j+1/2}^n ; \qquad (2.20)$$

where

$$\left(\frac{\Delta\sigma}{\Delta t}\right)^{n+1/2}_{j+1/2} = \frac{\sigma^{n+1}_{j+1/2} - \sigma^{n}_{j+1/2}}{t^{n+1} - t^{n}} ;$$

$$\left(\frac{\Delta q}{\Delta t}\right)^{n}_{j+1/2} = \frac{q^{n+1/2}_{j+1/2} - q^{n-1/2}_{j+1/2}}{t^{n+1/2} - t^{n-1/2}} ;$$

and

$$\left[(a^{+})^2\right]^{n+}_{j+1/2} = \left(a^{n}_{j+1/2}\right)^2 + (\Gamma\rho q)^{n+1/2}_{j+1/2} .$$

The WONDY difference scheme for (2.7) is given by:

$$\left(\frac{\Delta\mathcal{E}}{\Delta t}\right)^{n+1/2}_{j+1/2} = -\sigma^{n+1/2}_{j+1/2}\left(\frac{\Delta V}{\Delta t}\right)^{n+1/2}_{j+1/2} ; \qquad (2.21)$$

where

$$\left(\frac{\Delta\mathcal{E}}{\Delta t}\right)^{n+1/2}_{j+1/2} = \frac{\mathcal{E}^{n+1}_{j+1/2} - \mathcal{E}^{n}_{j+1/2}}{t^{n+1} - t^{n}} ;$$

and

$$\sigma^{n+1/2}_{j+1/2} = (\sigma^{n+1}_{j+1/2} + \sigma^{n}_{j+1/2})/2 .$$

3. LEMMAS

In Section Four certain 2 by 2 amplification matrices arise and their eigenvalues are roots of certain quadratic equations; i.e.,

$$\lambda^2 - 2B\lambda + C = 0 .$$

The Lemmas in this section are used to arrive at the timestep restrictions of Section Four.

Lemma 1A

Let B and C be real numbers; $D = B^2 - C$; $\lambda_\pm = B \pm D^{1/2}$; and $|\lambda|_{max} = \max(|\lambda_+|, |\lambda_-|)$.

<u>Case (a)</u>: If $D \geq 0$ and $B^2 > 1$, then

$$|\lambda|_{max} > 1 .$$

<u>Case (b)</u>: If $D \geq 0$ and $B^2 \leq 1$, then

$$[|\lambda|_{max} \leq 1 \text{ iff } 2|B| \leq C + 1] .$$

<u>Case (c)</u>: If $D < 0$, then

$$[|\lambda|_{max} \leq 1 \text{ iff } C \leq 1] .$$

Moreover, the result also holds when $\leq$ is replaced by $<$ or by $=$ inside the square brackets.

<u>Proof</u>:

<u>Case (a)</u>: If $D \geq 0$, then $|\lambda|_{max} = |B| + D^{1/2}$. If $|B| > 1$, then $|\lambda|_{max} > 1$.

<u>Case (b)</u>: $|B| + D^{1/2} \leq 1$ iff $B^2 - C \leq (1 - |B|)^2$ iff $2|B| \leq C + 1$.

Case (c): If $D < 0$, then λ_+ and λ_- are complex conjugates and

$$\lambda_+\lambda_- = |\lambda|^2_{max} = C.$$

End of proof.

Lemma 1B

If $B = 1 - b$, $C = 1 - c$, and $2b \geq c \geq 0$, then

$$|\lambda|_{max} \leq 1 \text{ iff } 2b + c \leq 4 .$$

Proof:

Case (b): First consider the subcase when $B > 0$. By Lemma 1A, $|\lambda|_{max} \leq 1$ iff $c \leq 2b$. Next consider the subcase when $B \leq 0$. By Lemma 1A, $|\lambda|_{max} \leq 1$ iff $2b + c \leq 4$.

Case (c) ($D < 0$): Since $C = 1 - c$ and $c \geq 0$, therefore, $C \leq 1$. By Lemma 1A, $C \leq 1$ iff $|\lambda|_{max} \leq 1$. This establishes that under the hypotheses of Lemma 1B, $2b + c \leq 4$ implies $|\lambda|_{max} \leq 1$ when $D < 0$. Now let's establish the reverse implication. $D < 0$ iff $2b + c < (4 - b)b$ and $(4 - b)b \leq 4$ for all real b. This establishes that under the hypotheses of Lemma 1B, $|\lambda|_{max} \leq 1$ implies $2b + c \leq 4$ when $D < 0$. End of proof.

Lemma 2

Assume A real, B and α positive; let $D = B^2 + A$; and let $\alpha' = \alpha(B + D^{1/2})$. Consider the following inequalities

$$[A\alpha^2 + 2B\alpha \leq 1] \tag{1}$$

and

$$[\alpha' \leq 1] . \tag{2}$$

Case (a): If $D \geq 0$, then (1) iff (2).

Case (b): If $D < 0$, then (1) holds for all real α.

Moreover the result also holds if the ≤ is replaced by < or by = inside the square brackets.

Proof:

Let $P(\alpha) = A\alpha^2 + 2B\alpha - 1$.

Case (a): First, consider the subcase A = 0. In this subcase it is easily seen that (1) iff (2). Second, consider the subcase A > 0. The larger of the two roots of $P(\alpha)$ is

$$\alpha_+ = \frac{-B + D^{1/2}}{A} = \frac{1}{B + D^{1/2}} .$$

Therefore, $P(\alpha) \le 0$ iff $\alpha \le \alpha_+$ and this shows that (1) iff (2). Third, consider the subcase A < 0. The smaller of the two roots of $P(\alpha)$ is

$$\alpha_- = \frac{-B + D^{1/2}}{A} = \frac{1}{B + D^{1/2}} .$$

Therefore, $P(\alpha) \le 0$ iff $\alpha \le \alpha_-$ and this shows that (1) iff (2).

Case (b): If D < 0, then $P(\alpha)$ has no real roots and thus $P(\alpha) < 0$ for all real α.

End of proof.

Lemma 3A (von Neumann's necessary condition)

Let the amplification matrix for the Fourier component of index k be denoted $\underset{\sim}{G}(\Delta t,k)$ where Δt is the time increment. Suppose $\underset{\sim}{G}(\Delta t,k)$ is an n by n matrix with its eigenvalues so labeled that

$$|\lambda_n| \le \cdots \le |\lambda_2| \le |\lambda_1| .$$

A necessary condition for stability is the condition

$$|\lambda_1| \le 1 + O(\Delta t)$$

for all k.

Proof:

The proof of this lemma may be found on page 70 of [2]. However, to make this report more self-contained that proof is reproduced here.

Let $R(\Delta t,k)$ be the spectral radius of $\underset{\sim}{G}(\Delta t,k)$. Recall that $R(\Delta t,k) \le \|\underset{\sim}{G}(\Delta t,k)\|$. It follows that a necessary condition for stability is: There exist constants C_1 and τ such that

$$R(\Delta t,k)^n \le C_1$$

for all Δt in $(0,\tau)$, for all n such that $0 \le n\Delta t \le t$ (where t is the final time), and for all k. Without loss of generality assume that $C_1 \ge 1$. The above inequality can be rewritten as

$$R(\Delta t,k) \le C_1^{\Delta t/t} .$$

Note that for $0 < \Delta t < \tau$, $C_1^{\Delta t/t} \le 1 + C_2\Delta t$ where $C_2 \ge (C_1^{\tau/t} - 1)/\tau$. Therefore, a necessary condition for stability is

$$R(\Delta t,k) \le 1 + O(\Delta t)$$

End of proof.

Lemma 3B (Sufficient Condition)

Let Δ be the determinant of the normalized eigenvectors of $\underset{\sim}{G}(\Delta t,k)$. If there exist constants δ and τ such that $|\Delta| \ge \delta > 0$ for all Δt in $(0,\tau)$ and for all k, then the von Neumann condition is sufficient for stability.

Proof:

The proof may be found on page 84 of [2]. However, to make this report more self-contained that proof is reproduced here.

Under the above hypotheses there exists a complete set of eigenvalues for $\underset{\sim}{G}$. Let $\underset{\sim}{E}$ be the matrix whose columns are the normalized right eigenvectors of $\underset{\sim}{G}$. Then $\underset{\sim}{E}^{-1}\underset{\sim}{G}\underset{\sim}{E} = \underset{\sim}{\Lambda}$ where

$$\underset{\sim}{\Lambda} = \begin{bmatrix} \lambda_1 & & 0 \\ & \lambda_2 & \\ 0 & & \lambda_m \end{bmatrix}$$

with $\lambda_1, \lambda_2, \ldots \lambda_m$ being the eigenvalues of $\underset{\sim}{G}$. Since the norm of any m by m matrix does not exceed m times the magnitude of its largest element, it follows that $\|\underset{\sim}{E}\| \le m$. Now

$$\underset{\sim}{E}^{-1} = \mathrm{cof}(\underset{\sim}{E})^T/\Delta$$

where $\Delta = \det(\underset{\sim}{E})$ and $\mathrm{cof}(\underset{\sim}{E})^T$ is the transpose of the cofactor matrix of $\underset{\sim}{E}$. Recall that $\mathrm{cof}(\underset{\sim}{E})_{ij}$ is the determinant of the cofactor of $(\underset{\sim}{E})_{ij}$. Since the absolute value of any determinant is bounded by the product of the lengths of its column (or row) vectors, it follows that

$$\|\underset{\sim}{E}^{-1}\| \le m/|\Delta| .$$

Now

$$\underset{\sim}{G} = \underset{\sim}{E}\,\Lambda\,\underset{\sim}{E}^{-1}$$

so

$$\underset{\sim}{G}^n = \underset{\sim}{E}\,\Lambda^n\,\underset{\sim}{E}^{-1}$$

therefore

$$\|\underset{\sim}{G}^n\| \le \|\underset{\sim}{E}\|\|\underset{\sim}{\Lambda}^n\|\,\|\underset{\sim}{E}^{-1}\| \le m^2R^n/|\Delta| .$$

Hence, the norm of $\underset{\sim}{G}^n$ is bounded provided Δ is bounded away from zero and $R \leq 1 + O(\Delta t)$. End of proof.

<u>Remark</u>: Note that Lemmas 3A and 3B have only been proved for linear difference equations with constant coefficients.

4. RESULTS

Remark: Stability is defined to be boundedness of the solutions to the equations of first variation. The equations of first variation are linear but they may have variable coefficients. If those coefficients are held constant, then the resultant equations are called the localized equations of first variation. Stable in the sense of von Neumann or von Neumann stability is defined to be boundedness of the solutions of the localized equations of first variation. It has been conjectured but not proved in general that von Neumann stability implies stability.

The first step in the von Neumann stability analysis is to calculate the equations of first variation of the difference equations. The WONDY difference equation for conservation of momentum is given by:

$$\left(\frac{\Delta u}{\Delta t}\right)_j^n = -\left(\frac{\Delta\sigma}{\Delta\mu}\right)_j^n . \tag{4.1}$$

To calculate the equation of first variation of Eqn. (4.1): replace u by $u + \delta u$ (following von Neumann-Richtmyer [1] notation) and σ by $\sigma + \delta\sigma$ in (4.1) and call it (4.1)′; subtract (4.1) from (4.1)′; neglect any terms of ordcr two or higher in δu and $\delta\sigma$ to get

$$\Delta(\delta u)/\Delta t = -\Delta(\delta\sigma)/\Delta\mu . \tag{4.2}$$

The uniform superscripts (n) and the uniform subscripts $(j + 1/2)$ have been suppressed. The WONDY difference relation for a rate dependent material relation of the form

$$\frac{\partial\sigma}{\partial t} + (a^+)^2 \frac{\partial V}{\partial t} - \frac{\partial q}{\partial t} = 0 \tag{4.3}$$

is

$$\left(\frac{\Delta\sigma}{\Delta t}\right)^{n+1/2}_{j+1/2} = -\left[(a^+)^2\right]^{n+}_{j+1/2}\left(\frac{\Delta u}{\Delta\mu}\right)^{n+1/2}_{j+1/2} + \left(\frac{\Delta q}{\Delta t}\right)^{n}_{j+1/2} . \tag{4.4}$$

Recall that

$$(a^+)^2 = a^2 + \Gamma\rho q . \tag{4.5}$$

The equation of first variation of Eqn. (4.4) is, in general, rather messy. Some assumptions are made to reduce the mess and simplify the analysis. Assume that the increments $\Delta t^{n+1/2}$ and $\Delta\mu_{j+1/2}$ are uniform in n and j; therefore, the super- and subscripts thereon may be suppressed. Next let's make some assumptions to simplify the form of q and a^+.

<u>Assumptions on the Stress Rate-Strain Rate Relations</u>: In the first analysis let's assume that q is given by:

$$q = -K_1\Delta\mu\left(\frac{\Delta u}{\Delta\mu}\right) ; \tag{4.6}$$

where K_1 is a positive constant. Also let's simplify a^+ to

$$(a^+)^2 = (a^o)^2 + b^o q \tag{4.7}$$

where a^o and b^o are positive constants with

$$b^o = (\Gamma\rho)^o . \tag{4.8}$$

These simplifying assumptions reduce the problem to considering only Eqns. (4.1) and (4.4). From Eqns. (4.1) and (4.6) it follows that

$$\frac{\Delta q}{\Delta t} = K_1\Delta\mu\,\frac{\Delta^2\sigma}{\Delta\mu^2} \tag{4.8}$$

and therefore (4.4) becomes

$$\left(\frac{\Delta\sigma}{\Delta t}\right)_{j+1/2}^{n+1/2} = -(a^o)^2 \left(\frac{\Delta u}{\Delta\mu}\right)_{j+1/2}^{n+1/2} + \Delta\mu\{\cdot\} \tag{4.9}$$

where

$$\{\cdot\} = \left\{b^o K_1 \left[\left(\frac{\Delta u}{\Delta\mu}\right)_{j+1/2}^{n+1/2}\right]^2 + K_1\left(\frac{\Delta^2\sigma}{\Delta\mu^2}\right)_{j+1/2}^{n}\right\} . \tag{4.10}$$

The equation of first variation of (4.10) is given by:

$$[\Delta(\delta\sigma)/\Delta t]^{n+1/2} = -(a^o)^2[\Delta(\delta u)/\Delta\mu]^{n+1/2} + \Delta\mu\delta\{\cdot\} \ ; \tag{4.11}$$

with

$$\delta\{\cdot\} = \left\{2K_1 b^o \left(\frac{\Delta u}{\Delta\mu}\right)^{n+1/2} [\Delta(\delta u)/\Delta\mu]^{n+1/2} + K_1[\Delta^2(\delta\sigma)/\Delta\mu^2]^n\right\} .$$

The uniform subscripts $(j+1/2)$ in the above are suppressed; the differing superscripts (n and $n+1/2$) are retained. Let

$$(a_1^+)^2 = (a^o)^2 + 2q\Gamma\rho \tag{4.12}$$

with q defined by (4.6); where $\Gamma\rho$ is held constant at b^o; then (4.11) can be written

$$[\Delta(\delta\sigma)/\Delta t]^{n+1/2} = -(a_1^+)^2[\Delta(\delta u)/\Delta\mu]^{n+1/2}$$

$$+ K_1\Delta\mu[\Delta^2(\delta\sigma)/\Delta\mu^2]^n . \tag{4.13}$$

The next step in the von Neumann stability analysis is to find the amplification matrix of the local equations of first variation. The local equations of first variation for the jth zone and nth cycle are just the equations of first variation with their coefficients fixed at their evaluations in the jth zone and nth cycle. Thus the next step is to do a Fourier series analysis on (4.2) and (4.13) with a_1^+ held constant. Substitute

$$(\delta\sigma)^n_{j+1/2} = -a_1^+ \, w^n \, \xi^{j+1/2} \tag{4.14}$$

and

$$(\delta u)^{n+1/2}_j = v^{n+1} \, \xi^j \tag{4.15}$$

with

$$\xi = \exp(ik\Delta\mu) \tag{4.16}$$

into (4.2) and (4.13). Let

$$\alpha = a_1^+ \, \Delta t/\Delta\mu \tag{4.17}$$

and

$$\beta = 2\alpha \, \sin \, k \, \Delta\mu/2 \tag{4.18}$$

then (4.2) becomes

$$v^{n+1} - v^n + i\beta w^n \tag{4.19}$$

and (4.13) becomes

$$w^{n+1} = i\beta v^{n+1} = w^n(1 - C_1) \tag{4.20}$$

where

$$C_1 = \frac{K_1 \Delta t}{\Delta\mu} \, (2 \, \sin \, k \, \Delta\mu/2)^2 \, .$$

Let

$$\vec{U} = \begin{bmatrix} v \\ w \end{bmatrix} \tag{4.21}$$

then (4.19) and (4.20) may be written in the form

$$\underset{\sim}{H}_1 \, \vec{U}^{n+1} = \underset{\sim}{H}_o \, \vec{U}^n$$

where

$$\underset{\sim}{H}_1 = \begin{bmatrix} 1 & 0 \\ -i\beta & 1 \end{bmatrix} \qquad (4.22)$$

and

$$\underset{\sim}{H}_o = \begin{bmatrix} 1 & i\beta \\ 0 & 1 - C_1 \end{bmatrix} . \qquad (4.23)$$

Let $G = \underset{\sim}{H}_1^{-1} \underset{\sim}{H}_o$ and (4.22) becomes

$$\vec{U}^{n+1} = \underset{\sim}{G} \vec{U}^n \qquad (4.24)$$

with the amplification matrix given by

$$\underset{\sim}{G} = \begin{bmatrix} 1 & i\beta \\ i\beta & 1 - \beta^2 - C_1 \end{bmatrix} . \qquad (4.25)$$

Consider the eigenvalues of $\underset{\sim}{G}$. Note that

$$\det(\underset{\sim}{G} - \lambda\underset{\sim}{I}) = \lambda^2 - 2(1 - b_1)\lambda + 1 - c_1 \qquad (4.26)$$

where

$$2b_1 = \beta^2 + c_1 \qquad (4.27)$$

and

$$c_1 = \frac{4K_1 \Delta t}{\Delta\mu} (\sin k\, \Delta\mu/2)^2 . \qquad (4.28)$$

<u>Result #1</u>:

Assume that a rate dependent relation of the form

$$\frac{\partial\sigma}{\partial t} + (a_1^+)^2 \frac{\partial V}{\partial t} - \frac{\partial q}{\partial t} = 0$$

is differenced in WONDY (as in (4.4)) with $(a_1^+)^2$ a real (but not necessarily positive) constant and

$$q = -K_1 \Delta\mu \left(\frac{\Delta u}{\Delta\mu}\right)$$

where $K_1 > 0$ is a constant. Then a necessary condition for stability is

$$(a_1^+)^2 r^2 + 2K_1 r \le 1 , \qquad (4.29)$$

where $r = \Delta t/\Delta\mu$.

Proof: Note that (4.29) is equivalent to : for all k

$$2b_1 + c_1 \le 4 . \qquad (4.30)$$

By Lemma 1B, $|\lambda_\pm| \le 1$ iff (4.30) for all k. Thus by Lemma 3A (4.29) is necessary. End of proof.

Result #2:

If $(a_1^+)^2 > 0$ and $0 < K_1 r < \alpha(1 - \alpha)$ where $\alpha = a_1^+ r$, then

$$\alpha^2 + 2K_1 r \le 1 \qquad (4.31)$$

is necessary and sufficient for stability.

Proof:

Necessity was established in Result #1. Now let's establish sufficiency. Let $B = 1 - b_1$; $C = 1 - c_1$; $D = B^2 - C$; $\lambda_\pm = B \pm D^{1/2}$; $\rho_\pm^2 = \beta^2 + |1 - \lambda_\pm|^2$; $v_1^\pm = -i\beta/\rho_\pm$ and $v_2^\pm = (1 - \lambda_\pm)/\rho_\pm$. Note that $\{\underset{\sim}{v}^+, \underset{\sim}{v}^-\}$ is a complete set of normalized right eigenvectors of $\underset{\sim}{G}$. Observe that

$$|\det(\underset{\sim}{v}^+, \underset{\sim}{v}^-)|^2 = 4\beta^2 |D| / (\rho_+ \rho_-)^2 . \qquad (4.32)$$

The idea is to show that there exsits a $\delta > 0$ such that

$$4\beta^2 |D| \geq \delta(\rho_+\rho_-)^2 \qquad (4.33)$$

then apply Lemma 3B. The next step is to show that $0 < K_1 r < \alpha(1 - \alpha)$ implies $D \leq 0$. Note that

$$D = -\beta^2\{1 - g(\beta^2)\}$$

where

$$g(\beta^2) = \frac{\beta^2}{4}\left(1 + \frac{K_1}{a\alpha}\right)^2$$

and observe that

$$g(\beta^2) < 1$$

is equivalent to

$$K_1 r < \alpha(1 - \alpha) \qquad (4.34)$$

This establishes $D \leq 0$. When $D \leq 0$, then

$$\rho_\pm^2 = 2\beta^2$$

and (4.33) reduces to

$$1 - g(\beta^2) \geq \delta .$$

Hence, (4.32) requires $g(\beta^2) < 1$; this has already been shown. End of proof.

Result #3:

If (4.34a) is enforced, then (4.29) is necessary and sufficient for stability.

Proof: The proof of Result #3 follows the same pattern as the proof of Result #2. End of proof.

In the next stability analysis let's complicate matters a bit by considering a viscosity coefficient of the von Neumann-Richtmyer-Landshoff form; i.e., let

$$q = -K_2 \Delta\mu \left(\frac{\Delta u}{\Delta\mu}\right) \tag{4.35}$$

with

$$K_2 = \Lambda_1 + \Lambda_2 \Delta\mu \left|\frac{\Delta u}{\Delta\mu}\right| \tag{4.36}$$

where Λ_1 and Λ_2 are positive constants. Note that

$$\frac{\Delta q}{\Delta t} = K_2^+ \Delta\mu \, \frac{\Delta^2 \sigma}{\Delta\mu^2} \tag{4.37}$$

where

$$K_2^+ = \Lambda_1 + 2\Lambda_2 \Delta\mu \left|\frac{\Delta u}{\Delta\mu}\right| . \tag{4.38}$$

Therefore (4.4) is altered to

$$\left(\frac{\Delta\sigma}{\Delta t}\right)_{j+1/2}^{n+1/2} = -(a^o)^2 \left(\frac{\Delta u}{\Delta\mu}\right)_{j+1/2}^{n+1/2} + \Delta\mu\{\cdot\}_2 \tag{4.39}$$

where

$$\{\cdot\}_2 = \left\{ b^o K_2 \left[\left(\frac{\Delta u}{\Delta\mu}\right)^{n+1/2}\right]^2 + K_2^+ \left(\frac{\Delta^2\sigma}{\Delta\mu^2}\right)^n \right\} . \tag{4.40}$$

The equation of first variation of (4.39) is given by:

$$[\Delta(\delta\sigma)/\Delta t]^{n+1/2} = -(a^o)^2[\Delta(\delta u)/\Delta\mu]^{n+1/2} + \Delta\mu\delta\{\cdot\}_2 \; ; \qquad (4.41)$$

with

$$\delta\{\cdot\}_2 = \left\{K_3[\Delta(\delta u)/\Delta\mu]^{n+1/2} + K_2^+[\Delta^2(\delta\sigma)/\Delta\mu^2]^n\right\}$$

where

$$K_3 = \mathrm{sign}\left(\frac{\Delta u}{\Delta\mu}\right)\left[b^o\left(2\Lambda_1 + 3\Lambda_2\Delta\mu \left|\frac{\Delta u}{\Delta\mu}\right|\right)\frac{\Delta u}{\Delta\mu} + 2\Lambda_2\Delta\mu\,\frac{\Delta^2\sigma}{\Delta\mu^2}\right] .$$

Let

$$(a_2^+)^2 = (a^o)^2 - \Delta\mu K_3 \; . \qquad (4.42)$$

Now (4.41) can be written

$$[\Delta(\delta\sigma)/\Delta t]^{n+1/2} = -(a_2^+)^2[\Delta(\delta u)/\Delta\mu]^{n+1/2} + K_2^+\Delta\mu[\Delta^2(\delta\sigma)/\Delta\mu^2]^n \; . \qquad (4.43)$$

The next step in the von Neumann stability analysis is to hold $(a_2^+)^2$ and K_2^+ constant and find the amplification matrix associated with (4.43) and (4.2). Of course, this is already done because (4.43) has the same form as (4.13). Thus Results #1, 2, and 3 hold with $(a_1^+)^2$ replaced by $(a_2^+)^2$ and K_1 replaced by K_2^+.

Let's define von Neumann stability or stable in the sense of von Neumann and then the results can be stated in a more convenient form.

Definition (von Neumann Stability)

Let $\vec{C} = (C_1,\ldots,C_m)$ be the coefficients of the equations of first variation of the difference equations. In general, the coefficients will depend on μ_j and t^n through the solutions to the difference equations. Suppose that the local equations of first variation at (μ_j,t^n) are stable under the timestep restriction

$$f(r,\vec{C}(\mu_j,t^n)) \leq 1 \ . \qquad (4.44)$$

Here f is some function of the coefficients $\vec{C}$ and $r = \Delta t/\Delta\mu$. If (4.44) holds for all j and n, then the difference scheme is said to be stable in the sense of von Neumann or von Neumann stable.

With the foregoing definition Results #1 and 3 may be summarized in the following.

Result #4:

Assume a rate dependent material relation of the form

$$\frac{\partial p}{\partial t} + (a^+)^2 \frac{\partial V}{\partial t} = 0$$

where

$$(a^+)^2 = (a^o)^2 + (\Gamma\rho)^o q$$

with a^o and $(\Gamma\rho)^o$ being positive constants. Suppose that

$$q = -K_2\Delta\mu \frac{\Delta u}{\Delta\mu}$$

where

$$K_2 = \Lambda_1 + \Lambda_2\Delta\mu \left|\frac{\Delta u}{\Delta\mu}\right|$$

with Λ_1 and Λ_2 being positive constants. Let the foregoing material relation be differenced in WONDY (as in (4.4)) with the restriction

$$0 < 2K_2^+ r < 1 \tag{4.45}$$

enforced where K_2^+ is defined by (4.38). A necessary and sufficient condition for von Neumann stability is

$$(a_2^+)^2 r^2 + 2K_2^+ r \leq 1 \tag{4.46}$$

where $(a_2^+)^2$ is given by (4.42).

Proof: The proof is the same as the proofs of Results #1 and #2 with $(a_1^+)^2$ replaced by $(a_2^+)^2$ and K_1 replaced by K_2^+. End of proof.

Remark: Result #4 may sound stronger than is warranted if one does not carefully note that only "von Neumann stability" is claimed.

5. SUMMARY, CONCLUSIONS, AND RECOMMENDATIONS

Before giving the summary, it should help the reader if a quick review of the notation and nomenclature is presented.

The von Neumann-Richtmyer-Landshoff artificial viscosity q in WONDY has the form

$$q = -\Delta\mu\left(\Lambda_1^o a + \Lambda_2^o \rho\Delta\mu \left|\frac{\Delta u}{\Delta\mu}\right|\right)\frac{\Delta u}{\Delta\mu}$$

where Λ_1^o and Λ_2^o are positive constants with $\Lambda_1^o \approx 0.1$ and $\Lambda_2^o \approx 1.0$. It is convenient to let

$$\Lambda = \Lambda_1^o a + \Lambda_2^o \rho\Delta\mu \left|\frac{\Delta u}{\Delta\mu}\right| .$$

Recall that: a is the acoustic impedance; ρ is the mass density; Δμ is the material increment ($\Delta\mu = \rho^o \Delta X$); and u is the specific momentum.

In WONDY the timestep restriction currently used is

$$r\left[\Lambda + \sqrt{a^2 + \Lambda^2}\right] < 1 \qquad (5.1)$$

where

$$r = \Delta t/\Delta\mu$$

and Δt is the timestep.

Assume that a non-isentropic equation of state is given. That is, assume that the pressure p is given as a function of the specific volume V and the specific internal energy $\mathcal{E}$ or as a function of V and the specific entropy S. In other words, some function $p_{V\mathcal{E}}$ or p_{VS} is given such that $p = p_{V\mathcal{E}}(V,\mathcal{E})$ or $p = p_{VS}(V,S)$ is the prescription for the pressure. Then since

$$a^2 = -\partial p_{VS}/\partial V$$

and

$$\Gamma\rho = \partial p_{V\mathcal{E}}/\partial\mathcal{E}$$

(where Γ is the Grüneisen parameter) it follows that (see Section Two for the details of the derivation)

$$\frac{\partial p}{\partial t} = -(a^+)^2 \frac{\partial V}{\partial t}$$

where

$$(a^+)^2 = a^2 + \Gamma\rho q$$

is the augmented (or instantaneous) acoustic impedance. And this leads to a rate dependent relation of the form

$$\frac{\partial\sigma}{\partial t} + (a^+)^2 \frac{\partial V}{\partial t} - \frac{\partial q}{\partial t} = 0 \ . \qquad (5.2)$$

<u>Summary</u>: The von Neumann stability analysis done in Section Four (and summarized in Result #4) suggests: when WONDY is using a non-isentropic material relation of the form $p = p_{V\mathcal{E}}(V,\mathcal{E})$ or $p = p_{VS}(V,S)$ (which leads to a rate dependent relation of the form (5.2)) then (5.1) should be modified to

$$r\left[\Lambda_3 + \sqrt{a_3^2 + \Lambda_3^2}\right] < 1 \qquad (5.3)$$

where

$$\Lambda_3 = \Lambda_1^o a + 2\Lambda_2^o \rho\Delta\mu \left|\frac{\Delta u}{\Delta\mu}\right|$$

and

$$a_3^2 = \max(0, a_2^2)$$

with

$$a_2^2 = a^2 - \Delta\mu \ \text{sign}\left(\frac{\Delta u}{\Delta\mu}\right)\left[K_4 \left|\frac{\Delta u}{\Delta\mu}\right| + K_5 \frac{\Delta^2\sigma}{\Delta\mu^2}\right]$$

where

$$K_4 = \Gamma\rho\left[2\Lambda_1^o a + 3\Lambda_2^o \rho\Delta\mu \left|\frac{\Delta u}{\Delta\mu}\right|\right]$$

and

$$K_5 = 2\Lambda_2^o \rho\Delta\mu \ .$$

Conclusion: The timestep restriction now in WONDY (5.1) may not be sufficient for stability in certain regions of certain calculations.

Recommendations: The timestep restriction in WONDY should be altered from inequality (5.1) to inequality (5.3).

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