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BRIEF COMMUNICATION

CAUSALITY VIOLATION OF COMPLEX-CHARACTERISTIC TWO-PHASE FLOW EQUATIONS

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1. INTRODUCTION

The use of two-phase flow models with unequal velocities and/or temperature has considerably expanded in nuclear safety analysis in recent years. It was soon pointed out that, in some of these models, the basic partial differential equations (pde's) have complex characteristics and—extrapolating from the realm of linear analysis—it was argued that this feature was the ultimate source of instabilities encountered in numerical computation (Lyczkowski *et al.* 1978).

Clearly, the discussion has so far focused on the mathematical, or rather, numerical question of *stability*. This paper wishes to discuss a physical argument based on *causality*. Specifically, we shall show (without making linear approximations) that accurate computation of the solution, at some time t, of the quasi-linear, complex-characteristic, two-phase flow equations requires the knowledge of the solution at all future times ($t' > t$). Thus, regardless of whether the numerical schemes representing these pde's are stable, one is faced with the choice of either building a numerical scheme *not* representative of the pde's or to violate a fundamental postulate of physics.

Most two-phase flow models can be written in terms of first-order quasi-linear equations of the form:

$$A\frac{\partial \boldsymbol{U}}{\partial t} + B\frac{\partial \boldsymbol{U}}{\partial x} = C\boldsymbol{U} + \boldsymbol{D} \qquad [1]$$

where $\boldsymbol{U}$ is an n-dimensional of the n dependent variables of the problem. $\boldsymbol{D}$ is also a n-dimensional source vector and A, B, and C are $n \times n$ matrices. It is usually possible, for two-phase flow equations, to reduce the system to one where A is a constant matrix, and B and C are functions of U but not explicit functions of x and t.

2. SMALL PERTURBATIONS—CAUSALITY REQUIREMENTS

In order to exhibit the connection between causality and complex characteristics we first consider a model where $C = 0$ and where small perturbations are added to a constant, uniform term:

$$\boldsymbol{U} = \boldsymbol{U}_0 + \boldsymbol{U}_1$$

$\boldsymbol{U}_0$ is a space-time independent term and $\boldsymbol{U}_1$ is assumed small compared to $\boldsymbol{U}_0$. Then, to first order in $\boldsymbol{U}_1$,[1] becomes:

$$A\frac{\partial \boldsymbol{U}_1}{\partial t} + B_0\frac{\partial \boldsymbol{U}_1}{\partial x} = \boldsymbol{D} \qquad [2]$$

where B_0 is the constant matrix, corresponding to B.

We now want to consider the Fourier spectral decomposition of U_1. Since, in real situations one encounters finite boundaries one should in fact use Fourier series for the *spatial* decomposition. We shall however assume that we are working in an infinite (one-dimensional) domain and use Fourier integrals. Let $u(x, t)$ be any component of U_1. We define its Fourier transform by:†

$$\tilde{U}(k, \omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{u}(x, t)\, \mathrm{e}^{-i(\omega t - kx)} \mathrm{d}x \mathrm{d}t \tag{3}$$

Equation [2] now becomes:

$$(i\omega A - ikB_0)\tilde{U}(k, \omega) = \tilde{D}(k, \omega).$$

Therefore, provided that the matrix or the l.h.s. is nonsingular, we obtain:

$$\tilde{U}(k, \omega) = [i\omega A - ikB_0]^{-1}\tilde{D}(k, \omega)$$

and finally; performing the inverse Fourier transform:

$$U(x, t) = \frac{1}{2\pi} \int [i\omega A - ikB_0]^{-1} \tilde{D}(k, \omega)\, \mathrm{e}^{i(\omega t - kx)}\, \mathrm{d}k\, \mathrm{d}\omega. \tag{4}$$

Defining now:

$$\tilde{G}(k, \omega) = [i\omega A - ikB_0]^{-1} \tag{5}$$

and

$$G(x, t) = \frac{1}{2\pi} \int \tilde{G}(k, \omega)\, \mathrm{e}^{i(\omega t - kx)}\, \mathrm{d}\omega\, \mathrm{d}k \tag{6}$$

the integral of [4] can be written as a convolution integral.

$$U(x, t) = \int_{-\infty}^{+\infty} G(x - x', t - t')\boldsymbol{D}(x', t')\, \mathrm{d}x'\, \mathrm{d}t'. \tag{7}$$

Now, it can readily be seen that, unless $G(x, t) = 0$ for $t < 0$, values of $\boldsymbol{D}(x', t')$ for $t' > t$ will influence the solution at t. Thus causality implies that the (Green) function‡ G is such that:

$$G(x, t) = 0 \text{ for } t < 0. \tag{8}$$

We shall not attempt to obtain an analytic form of $G(x, t)$. We only want to investigate the necessary and sufficient conditions to fulfill the causality requirements specified by [8]. Let us then integrate [6] over $\mathrm{d}\omega$ for a fixed value of k. This is done as follows: first, we analytically continue the integrand $G(k, \omega)\,\mathrm{e}^{i(\omega t - kx)}$ into the complex ω-plane; then we replace the integration on the real axis $(-\infty, +\infty)$ by a contour integration. The contour is defined by the real axis and a half circle at infinity (c). Symbolically, we write:

$$G(x, t) = \int \mathrm{d}\omega \equiv \int_{-\infty}^{+\infty} \mathrm{d}\omega + \int_{(c)} \mathrm{d}\omega \tag{9}$$

†A function $u(x, t)$ and its Fourier transform are designated with the same letter. They are distinguished from one another by their arguments and by a tilde (~).

‡Note that G is in fact a matrix. The discussion applies to each component G_{ij} of G.

In view of [6], this equation can only be valid if the integral over the half-circle at infinity is zero, that is, if the integrand vanishes there. Thus we consider two cases:

(a) $t > 0$. In this case, we take (c) as the half-circle in the *upper* half ω-plane. The integrand is zero on (c) because it behaves as limit of $\exp(-\mathrm{Im}(\omega)\, t)$, when $\mathrm{Im}(\omega) \to \infty$.

(b) $t < 0$. In this case, for the same reason, we take (c) in the *lower* half ω-plane. Now, Cauchy's theorem states that the value of the contour integral is equal to $2\pi i$ times the sum of the residues of the poles included inside the contour. Returning to [6], we see that the poles of the integrand occur whenever the determinant of the matrix $(i\omega A - ikB_0)$ is zero. On the other hand, the characteristics of the pdes are given by the roots of $\det(\lambda A - B_0)$. Thus, the poles in the ω-plane and the characteristics of the pdes are simply related by the real variable k: $\omega = k\lambda$. Finally, if the characteristics are complex, it is well known that they occur in complex conjugate pairs and therefore the integrand of the integral in [6] will have poles in both the upper and lower half ω-plane. The contour integral of [9], in such a case, will be non-zero for both $t > 0$ and $t < 0$. This result specifically violates the causality requirement of [8].

If, on the other hand, the roots of the determinant are real (i.e. hyperbolic system) then one cannot perform the contour integration immediately because the poles are on the contour itself. One can show however (see e.g. Feynman & Hibbs 1965)

$$\int_{-\infty}^{+\infty} \frac{f(\omega)\, e^{i\omega t}}{\omega - \omega_0}\, d\omega = \begin{cases} 0 \text{ for } t < 0 \\ 2i\pi f(\omega_0)\, e^{i\omega_0 t} \text{ for } t > 0. \end{cases} \qquad [10]$$

In conclusion we found that, at least for small perturbations, existence of complex characteristics would violate the requirement of causality. The result is well-known for the linear case. We now extend it to the general case.

3. THE GENERAL CASE

The objective here is *not* to solve the pdes but to exhibit the dependence of the solution of [1] on future events if some characterics are complex.

Let us start again from [1] and perform a space-time Fourier transformation on all nonconstant quantities. We get:

$$\int i\omega A\tilde{U}(k,\omega)\, e^{i(\omega t - kx)}\, d\omega\, dk - \int ik_2 \tilde{B}(k_1,\omega_1)\tilde{U}(k_2,\omega_2)$$

$$\times\, e^{i(\omega_1+\omega_2)t - i(k_1+k_2)x}\, d\omega_1\, d\omega_2\, dk_1\, dk_2 -$$

$$-\int \tilde{C}(k_1,\omega_1)\tilde{U}(k_2,\omega_2)\, e^{i(\omega_1+\omega_2)t - i(k_1+k_2)x}\, d\omega_1\, d\omega_2\, dk_1\, dk_2 =$$

$$= \int \tilde{D}(\omega,k)\, e^{i(\omega t - kx)}\, d\omega\, dk.$$

Next, we perform a change of dummy variable (k_2, ω_2) in the second and third integrals: $k = k_1 - k_2$, $\omega = \omega_1 - \omega_2$. We find after regrouping:

$$+\int d\omega dk\, e^{i(\omega t - kx)} \{im A\tilde{U}(k,\omega) - \int d\omega_1 dk_1 [i(k-k_1)\tilde{B}(k_1,\omega_1)$$

$$+ \tilde{C}(K_1,\omega_1)]\tilde{U}(k-k_1,\omega-\omega_1) - \tilde{D}(\omega,k)\} = 0.$$

Now, since $e^{i(\omega t - kx)}$ is a complete set of orthogonal functions, the term within wiggly brackets {}

must be null:

$$i\omega A\tilde{U}(k,\omega)-\int[i(k-k_1)\tilde{B}(k_1,\omega_1)+\tilde{C}(k_1,\omega_1)]\tilde{U}(k-k_1,\omega-\omega_1)\,\mathrm{d}k_1\,\mathrm{d}\omega_1$$
$$=\tilde{D}(k,\omega).$$

We now solve this equation for a specific spectral component $U(k, \omega)$ (i.e. with specific values of k and ω). That is, we extract from the integral the $U(k, \omega)$ corresponding to the first term and we get:

$$[i\omega A-ik\tilde{B}(o,o)-\tilde{C}(o,o]\tilde{U}(k,\omega)=\tilde{D}(k,\omega)+\tilde{E}(k,\omega) \qquad [11]$$

where

$$\tilde{E}(k,\omega)=\int[i(k-k_1)\tilde{B}(k_1,\omega_1)+\tilde{C}(k_1,\omega_1)]\tilde{U}(k-k_1,\omega-\omega_1)$$

$$\times[1-\delta(k_1,\omega_1)]\,\mathrm{d}\omega_1\,\mathrm{d}k_1$$

$\delta(k_1, \omega_1)$ is the Dirac delta function. Therefore, from [11]:

$$\tilde{U}(k,\omega)=[i\omega A-ik\tilde{B}(o,o)-\tilde{C}(o,o)]^{-1}(\tilde{D}(k,\omega)+\tilde{E}(k,\omega)) \qquad [12]$$

and finally, returning to (x, t) coordinates we obtain, as in the preceding section:

$$\boldsymbol{U}(x,t)=\int_{-\infty}^{+\infty}G(x-x',t-t')[\boldsymbol{D}(x',t')+\boldsymbol{E}(x',t')]\,\mathrm{d}x'\,\mathrm{d}t' \qquad [13]$$

where

$$G(x,t)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}[i\omega A-ik\tilde{B}(o,o)-\tilde{C}(o,o)]^{-1}\,\mathrm{e}^{i(\omega t-kx)}\,\mathrm{d}k\,\mathrm{d}\omega. \qquad [14]$$

The discussion of the preceding section remains valid. The existence of poles in both the upper and lower half ω-plane in the integral of [14], guaranteed by the presence of complex characteristics, would violate the causality condition of [8]. The existence of the matrix $\tilde{C}(o, o)$ in the determinant of $[i\omega A - ik\tilde{B}(o, o) - \tilde{C}(o, o)]^{-1}$ does not alter the conclusions. For let us suppose that some roots† of:

$$\det[\lambda A-\tilde{B}(o,o)]=o$$

are complex and occur in complex conjugate pairs. Then, by continuity, the roots of:

$$\det[i\omega A-ik\tilde{B}(o,o)-\tilde{C}(o,o)]=ik\det\left[\frac{\omega}{k}A-\tilde{B}(o,o)+\frac{i\tilde{C}(o,o)}{k}\right]$$

will also be complex for sufficiently large values of k, and will occur on both sides of the real ω-axis (although they would no longer occur in complex conjugate pairs). Depending on the structure of C, there may be a threshold k_c such that the poles are all in the upper half of the

†Although $B(x, t)$ and $\tilde{B}(o, o)$ are not identical matrices, it can be shown that if $\det(\lambda A - B(x, t) = o$ has complex roots then $\det(\lambda A - \tilde{B}(o, o)$ will also have complex roots provided the characteristics of the pdc's are complex almost everywhere.

ω-plane for $|k| < k_c$, however we should emphasize that this result is obtained for the basic equations themselves, not for their finite-difference approximations. Therefore, there is no reason, mathematical or physical, that we should assume a cut-off $k = k_c$ in the integral of [14]. The existence of complex characteristics is thus a sufficient condition to insure that at least large wavenumber phenomena violate causality, even taking into account non-linear features. On the other hand, the existence of a threshold k_c may help explain why this effect is sometimes suppressed in some (non-convergent) finite-difference representations.

4. CONCLUSIONS

The preceding analysis did not attempt to solve the basic pde's of two-phase-flow. Instead we considered a transformation of these equations that exhibited the link between characteristics of the equations and the causality constraints. We have shown that causality is violated unless the characteristics are all real. The proof is not based on the linearized equations but take full account of the quasi-linear structure of the pde's. The proof is valid for the basic equations themselves. Thus, any finite-difference representation of these equations will be either inaccurate or acausal.

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