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Error dynamics: A new paradigm in scientific computing

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ABSTRACT

The most widely used error and stability analysis is based on a method by von Neumann [1] and is based on the assumption that the signal and the error satisfy the same equation for linear differential equations. We establish that even for computing linear equation, the solution and error do not follow same dynamics - a very counter-intuitive result.

We focus here on a simple linear problem with an exact solution, so that the limits of accurate computations are understood. For this purpose, we look at the one-dimensional convection equation,

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0, \qquad c > 0, \tag{1}$$

that admits non-dispersive and non-dissipative solution convecting to the right with the phase speed c. Any inaccuracy of the computed solution is not due to nonlinearity. Using Fourier-Laplace transforms we write $u(x,t) = \int U(k,t)e^{ikx}dk$. A numerical amplification factor[2] is introduced as $G(k) = U(k, t+dt)/U(k,t)$, such that in the continuum limit one must have $|G(k)| = 1$ - a requirement of neutral stability. Also, for space-time dependent problems numerical group velocity (V_{gN}) must be equal to the physical group velocity and the numerical phase speed c_N must be equal to c. The general numerical solution of Eq. (1) is $\bar{u}_N = \int A_0(k)[|G|]^{t/\Delta t}e^{ik(x-c_N t)}dk$ for $A_0(k)$ as the initial amplitude. It is noted that $\bar{u}_N$ satisfies[2],

$$\frac{\partial \bar{u}_N}{\partial t} + c_N\frac{\partial \bar{u}_N}{\partial x} = -\int \frac{dc_N}{dk}\left[\int ik' A_0[|G|]^{t/\Delta t}e^{ik'(x-c_N t)}dk'\right]dk + \int \frac{Ln\,|G|}{\Delta t}A_0[|G|]^{t/\Delta t}e^{ik(x-c_N t)}dk \tag{2}$$

If one defines numerical error as $e = u - \bar{u}_N$, then it's governing equation is given by,

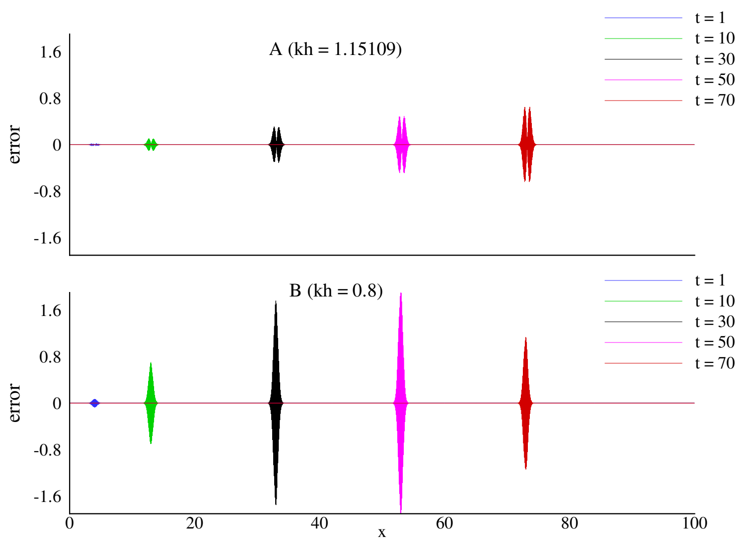
$$\frac{\partial e}{\partial t} + c\frac{\partial e}{\partial x} = -c[1 - \frac{c_N}{c}]\frac{\partial \bar{u}_N}{\partial x} - \int \frac{V_{gN} - c_N}{k}\left[\int ik' A_0[|G|]^{t/\Delta t}e^{ik'(x-c_N t)}dk'\right]dk - \int \frac{Ln\,|G|}{\Delta t}A_0[|G|]^{t/\Delta t}e^{ik(x-c_N t)}dk \tag{3}$$

Note that Eq. (3) is an exact equation - unlike the modified equation approaches[3], where the resultant equation depends on the method of discretization. In contrast, Eq. (3) clubs error based on generic numerical properties. For example, for a neutrally stable method, the last term is identically zero. This

establishes the futility of using stable methods, while demanding accuracy. The first term on the right hand side (RHS) of (3) is due to the phase error and the second term contributes to the spurious dispersion. To show the effect of Eq. (3) we solve (1) using $RK4$ for time integration and $OUCS3$ for spatial discretization[2]. Initial wave-packet is given by $u_0(x) = e^{-8(x-x_0)^2} cos(kx)$, where $x_0 = 6$ is the centre of the packet in physical space and kh ($h = \Delta x$) in the k- plane. Details of the cases performed are given below.

$Cases$	kh	$c\Delta t/h$	$\|G\|$	$\int \frac{(V_{gN} - c_N)}{k} dk$	$(1 - c_N/c)$
A	1.151	0.01	1	0.005	0.000
B	0.800	0.01	1	0.005	0.001

The contribution from dispersion error is the same for A and B. While A is chosen such that the phase error is negligibly small, for B it is higher. Computed errors for these two cases are shown in figure below. Error is present in both the cases, but it is more in B than in A. Presence of non-negligible error for A shows the effect of the dispersion error term exclusively, as the contribution from phase error is negligible, while no error is caused due to $|G| \neq 1$. The larger error for B shows the effect of phase error term in Eq. (3).



These two test cases clearly establish the need for a correct error analysis with proper role ascribed to individual sources- as shown on the RHS of Eq. (3).

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