TIME DEPENDENT CONVECTION-DIFFUSION

We now consider the equation $\frac{\partial \phi}{\partial t} + u \frac{\partial u}{\partial x} - \frac{\partial}{\partial x} \left(D \frac{\partial \phi}{\partial x} \right) = S$, with initial condition $\phi(x,0) = f(x)$ and appropriate boundary conditions Two new numerical difficulties arise that were not present before. These are *NUMERICAL DAMPING* and *NUMERICAL PHASE LAG* and we will illustrate them through the following example: Let us solve the advection equation $\frac{\partial \phi}{\partial t} + 0.25 \frac{\partial u}{\partial x} = 0$ in 0<x<2 with initial condition $\phi(x,0) = e^{-800(x-0.25)^2}$ and boundary conditions $\phi(0,t) = \phi(2,t) = 0$. We will apply the Crank-Nicolson-Galerkin ($\theta = 1/2$) method with 80 Linear elements, that is $\Delta x = 0.025$, and time step $\Delta t = 0.09$.





"NOISE" in the solution.





$$\oint = \sum_{n=-\infty}^{\infty} \Phi_n = \sum_{n=-\infty}^{\infty} c_n e^{i\alpha_n(x-at)}$$
The coefficients c_n and the wave numbers α_n depend on he initi
condition. Define the Analytical Amplification Factor (AAF) as
the ratio of the amplitude of the n-th Fourier component at time
 $t + \Delta t$ to the amplitude at time t. $AAF = \left| \frac{\Phi_n(x, t + \Delta t)}{\Phi_n(x, t)} \right|$. The
amplitude incresses, decreases or remains the same depending on
whether AAF is geater than, less than or equal to 1.
We can consider one component $\Phi_n = c_n e^{i\alpha_n[x-a(t+\Delta t)]}$, then the
AAF reduces to $AAF = \left| \frac{\Phi_n(x, t + \Delta t)}{\Phi_n(x, t)} \right| = \left| e^{i\alpha_n\Delta t} \right| = 1$
In the absence of numerical error, the solution must not change
the amplitude of the Fourier components in time.

To understand the behavior of the numerical solution, we write it				
as a discrete Fourier series $\phi(x_j, t_n) = \sum_{k=-K}^{n} a_k(t) \xi^n e^{i[k_k(j\Delta x)]}.$				
The coefficients a_k depend on the initial condition; ξ is a constan K is the number of elements contained in $0 < x < L$ (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the contained in $0 < x < L$) (one half of the containe	t; ie			
domain); $i = \sqrt{-1}$ and $k_k = \frac{2\pi\kappa}{2L}$ is a wave number.				
The corresponding frequencies are $f_k = \frac{k_k}{2\pi}$ and measure the number				
of wavelengths contained in each 2L interval. The lowest, $k = 0$, corresponds to a time independent term. The highest, $j = K$ has wave				
number $\frac{2\pi K}{2L} = \pi \left(\frac{K}{L}\right) = \frac{\pi}{\Delta x}$ and gives the number of points that will				
represent represent a sine wave between 0 and 2π .				
The finite series above is the exact solution generated by the numerical method when the a_k are the Fourier coefficients of				
the initial condition. 6				

The Numerical Amplification Factor is defined as $NAF = \begin{vmatrix} \phi_j^{n+1} \\ \phi_j^n \end{vmatrix} = |\xi|$ The DAMPING is the numerical error γ_d in the amplification factor for a component j. $\gamma_d = \frac{NAF}{AAF} = \frac{|\xi|}{1} = |\xi|.$ To propagate a solution without amplification error we need $|\xi| = 1$. **EXAMPLE** Discretize the convective equation $\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} = 0$ using the Crank-Nicolson-Galerkin method with linear elements. We obtain

 $\begin{bmatrix} h\\ 6\Delta t \begin{bmatrix} 2 & 1\\ 1 & 2 \end{bmatrix} + \frac{u}{4} \begin{bmatrix} -1 & 1\\ -1 & 1 \end{bmatrix} \begin{bmatrix} \phi_1^{n+1}\\ \phi_2^{n+1} \end{bmatrix} = \begin{pmatrix} h\\ 6\Delta t \begin{bmatrix} 2 & 1\\ 1 & 2 \end{bmatrix} - \frac{u}{4} \begin{bmatrix} -1 & 1\\ -1 & 1 \end{bmatrix} \begin{bmatrix} \phi_1^n\\ \phi_2^n \end{bmatrix}$

Assembling two elements the difference equation for node *j* is

$$\frac{2}{3} \Big[\left(\phi_{j-1}^{n+1} + 4\phi_{j}^{n+1} + \phi_{j+1}^{n+1} \right) - \left(\phi_{j-1}^{n} + 4\phi_{j}^{n} + \phi_{j+1}^{n} \right) \Big] + \frac{u\Delta t}{h} \Big[\left(\phi_{j+1}^{n+1} - \phi_{j-1}^{n+1} \right) + \left(\phi_{j+1}^{n} - \phi_{j-1}^{n} \right) \Big] = 0$$
Replace $\phi_{1}^{n} = \xi^{n} e^{i(k\cdot jh)}$

$$\frac{2}{3} \Big[\xi^{n+1} \left(e^{i(k\cdot j-1)h} + 4e^{ikjh} + e^{ik(j+1)h} \right) - \xi^{n} \left(e^{ik(j-1)h} + 4e^{ikjh} + e^{ik(j+1)h} \right) \Big]$$

$$+ \frac{u\Delta t}{h} \Big[\xi^{n+1} \left(e^{ik(j+1)h} - e^{ik(j-1)h} \right) + \xi^{n} \left(e^{ik(j+1)h} - e^{ik(j-1)h} \right) \Big] = 0$$
Multiply by ξ^{-n} , $\frac{3}{2}$, and $e^{-ik(j-1)h}$

$$(\xi - 1) \Big(1 + 4e^{ikh} + e^{i2kh} \Big) + \frac{3u\Delta t}{2h} (\xi + 1) \Big(e^{i2kh} - 1 \Big) = 0$$
Because kh can attain any value we set $\theta = kh$. Using Euler's equation we have $e^{i\theta} = \cos \theta + i\sin \theta$ and $e^{2i\theta} = (\cos \theta + i\sin \theta)^{2}$

 $(\xi - 1)\left(1 + 4(\cos\theta + i\sin\theta) + \cos^2\theta + 2i\cos\theta\sin\theta - \sin^2\theta\right) + \frac{3u\Delta t}{2h}(\xi + 1)\left((\cos\theta + i\sin\theta)^2 - 1\right) = 0$ Further manipulations yield $\xi(\cos\theta(4 + 2\cos\theta) + i\sin\theta(4 + 2\cos\theta)) - (\cos\theta(4 + 2\cos\theta) + i\sin\theta(4 + 2\cos\theta)) + i\frac{3u\Delta t}{h} \sin\theta(\cos\theta + i\sin\theta) = 0$ And finally $\xi = \frac{(4 + 2\cos\theta) - i\frac{3u\Delta t}{h} \sin\theta}{(4 + 2\cos\theta) + i\frac{3u\Delta t}{h} \sin\theta}$ **REMARKS:** 1) Noting that k is a wave number, $k = 2\pi/L$ if L is the wave length, then $\theta = kh = k\Delta x = 2\pi \left(\frac{\Delta x}{L}\right)$. This is convenient for us to plot the magnitude of ξ versus the number of elements per wave length in a covenient way. 2) The expression for ξ is of the form $\frac{\zeta}{z}$ therefore $|\xi| \equiv 1$ and the Crank-Nicolson-Galerkin method HAS NO DAMPING. This is good because the algorithm preserves the amplitude of the Fourier components, but it is bad because the method has no mechanism to eliminate perturbations. Moreover 3) We define the Courant number *c* as $c = \frac{u\Delta t}{h}$. If the mesh and time step are chosen so that c = 1, a particle of fluid will travel exactly the distance *h* in one time step. The peak translates from one node to the next and the solution is excellent. However, our introductory example has c = 0.9, and the results were disastrous. Therefore, the mesh could not capture the peak except every 10 time steps. The algorithm does one of two things: i) Assume that the peak is attained at the node closest to it, thus changing the speed of propagation and introducing phase lag. ii) Give the correct value at the closest node, and to conserve mass, redistribute the excess mass throughout the domain. Due to lack of memory (the method only knows what happens at $t = t_n$, but once the amplitude decreases it cannot increase back up. Thus producing damping and noise.

What actually happens is a combination of the two. This introduces dispersion and numerical damping. Moreover, because there is no damping in the algorithm ($|\xi| = 1$) there is no mechanism to kill the oscillations so they just stay there and as the amplitude continues to decay they eventually destroy the solution.

EXAMPLE

Apply the Petrov- Galerkin method with $\theta = 1$. The difference equation $\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} = 0$, use the θ -method with $\theta = 1$. The difference equation is $\phi_j^{n+1} + c \left(\phi_j^{n+1} - \phi_{j-1}^{n+1}\right) = \phi_j^n$ and replacing $\phi_j^n = \xi^n e^{ikjh}$ as before we obtain

$$\xi = \frac{1}{1 + c(1 - \cos\theta + i\sin\theta)}$$

from here we get
$$|\xi| = \left[(1 + c)^2 + c^2 - 2c(1 + c)\cos\theta \right]^{-1/2}$$



4) In this example $\theta = 1$, so the method is unconditionally stable. Because the NAF $|\xi|$ is less than 1, perturbations in the solution will decrease and eventually disappear in time. But if $|\xi| > 1$ perturbations will grow and and the algorithm become unstable. The stability is governed by

$$\xi \left| \begin{cases} <1 & stable \\ =1 & neutrally & stable \\ >1 & unstable \end{cases} \right|$$

This criterion for stability is only useful for linear equations, but it can be extended to systems of linear equations as well.

EXAMPLE

Let us now use $\theta = 0$ to discretize the convective equation. The difference equation is $\phi_j^{n+1} = c(\phi_{j-1}^n - \phi_j^n) + \phi_j^n$ fully explicit.



The phase angle of a Fourier component is given by $\tau = \tan^{-1} \left(\frac{\operatorname{Im}(\xi)}{\operatorname{Re}(\xi)} \right)$ In one time step, the real wave moves a distance τ_0 given by $\tau_0 = 2\pi/N$ where N is the number of time steps required to move one full wave length. Therefore, $N = \frac{L}{u\Delta t}$. Replacing in the expression for τ_0 we get $\tau_0 = c\theta$. The phase error Θ is defined as $\Theta = \tau_0 - \tau = c\theta - \tan^{-1} \left(\frac{\operatorname{Im}(\xi)}{\operatorname{Re}(\xi)} \right)$ **EXAMPLE** The phase angle for the explicit convective algorithm $\phi_j^{n+1} = c(\phi_{j-1}^n - \phi_j^n) + \phi_j^n$ is given by $\tau = \tan^{-1} \left(\frac{-c\sin\theta}{1 - c(1 - \cos\theta)} \right)$. The phase error Θ is shown in the figure.







In the steady-state case we added a balancing diffusion, and introduced a parameter α determined from the truncation error analysis.

We now introduce a second term and parameter to balance dispersion. $\begin{pmatrix} a^3 A \end{pmatrix}$

This has the form $\beta d\left(\frac{\partial^3 \phi}{\partial x^2 \partial t}\right)$, with $d \sim uh\Delta t$ for consistency. The modified equation is

$$\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} - \left(D + \frac{\alpha u h}{2} \right) \frac{\partial^2 \phi}{\partial x^2} + \beta d \frac{\partial^3 \phi}{\partial x^2 \partial t} = 0$$

Now we apply a Petrov-Galerkin method using linear space-time shape functions and the functions M_i as weights. Then the weak form is re-arranged as done before for the steady-state case and we obtain the final Petrov-Galerkin weights

$$w_i(x,t) = M_i(x,t) + \frac{\alpha h}{2} \frac{\partial M_i}{\partial x} + \frac{\beta h \Delta t}{4} \frac{\partial^2 M_i}{\partial x \partial t}_{_{19}}$$

The weighting functions become

$$\begin{split} w_{1}(x,t) &= 4 \left(1 - \frac{x}{h} \right) \frac{t}{\Delta t} \left(1 - \frac{t}{\Delta t} \right) - 2\alpha \frac{t}{\Delta t} \left(1 - \frac{t}{\Delta t} \right) - \beta \left(1 - \frac{2t}{\Delta t} \right) \\ w_{2}(x,t) &= 4 \frac{x}{h} \frac{t}{\Delta t} \left(1 - \frac{t}{\Delta t} \right) + 2\alpha \frac{t}{\Delta t} \left(1 - \frac{t}{\Delta t} \right) + \beta \left(1 - \frac{2t}{\Delta t} \right) \\ \int_{a}^{b} w \left(\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} - D \frac{\partial^{2} \phi}{\partial x^{2}} \right) dx = 0 \\ \end{split}$$
The difference equation for node *i* is

$$\begin{aligned} \frac{1}{9\Delta t} \left[\left(\phi_{i+1}^{n+1} - \phi_{i-1}^{n} \right) + 4 \left(\phi_{i}^{n+1} - \phi_{i}^{n} \right) + \left(\phi_{i+1}^{n+1} - \phi_{i+1}^{n} \right) \right] \\ &- \frac{\alpha}{6\Delta t} \left[\left(\phi_{i+1}^{n+1} - \phi_{i-1}^{n} \right) - \left(\phi_{i-1}^{n+1} - \phi_{i-1}^{n} \right) \right] + \frac{u}{6h} \left[\left(\phi_{i+1}^{n+1} + \phi_{i-1}^{n} \right) - \left(\phi_{i-1}^{n+1} + \phi_{i-1}^{n} \right) \right] \\ &- \left[\frac{u}{6h} (\alpha - \beta) + \frac{D}{3h^{2}} \right] \left(\phi_{i+1}^{n+1} - 2\phi_{i}^{n+1} + \phi_{i-1}^{n} \right) = 0 \end{aligned}$$

The truncation error is manipulated so that it is written in terms of coefficients of the derivatives
$$\phi_{xx}, \phi_{tx}, \phi_{txx}, \phi_{txx}, \dots$$
 Here $\phi_{txx} = \frac{\partial^3 \phi}{\partial t \partial x^2}$ etc.
The truncation error is
$$TE = \left(\frac{2D}{3\gamma}\right) (\sinh \gamma) \left[1 - \left(\alpha + \frac{2}{\gamma}\right) \tanh\left(\frac{\gamma}{2}\right) \right] (\phi_i^{n+1})_{xx} + \left(\frac{2h}{3\gamma^2}\right) \left[\sinh \gamma - \left(\alpha + \frac{2}{\gamma}\right) (\cosh \gamma - 1) \right] (\phi_i^{n+1})_{tx} + \left(\frac{h^2}{3}\right) \left[\frac{\alpha}{\gamma} + \frac{\beta c}{2} + \frac{2}{\gamma^3} \sinh \gamma \left(1 - \tanh\left(\frac{\gamma}{2}\right) \right) - \frac{4}{\gamma^4} (\cosh \gamma - 1) \right] (\phi_i^{n+1})_{txx} + \left(\frac{h^3}{3}\right) \left[\frac{c^2}{3} \left(\frac{1}{\gamma} - \frac{c - \alpha}{4}\right) - \frac{\alpha}{2} \left(\frac{1}{6} - \frac{c}{\gamma} - \frac{2}{\gamma^2}\right) - \frac{1}{6\gamma} + \frac{\beta c^2}{4} + \frac{2}{\gamma^4} \sinh \gamma \left(1 - \tanh\left(\frac{\gamma}{2}\right) \right) - \frac{4}{\gamma^5} (\cosh \gamma - 1) \right] (\phi_i^{n+1})_{txx} + HOT$$

Notice that
$$\beta$$
 does not appear in the first two terms. Moreover
choosing $\alpha = \operatorname{coth}\left(\frac{\gamma}{2}\right) - \frac{2}{\gamma}$ the same as before in the steady state
case, the first two terms vanish and the error reduces to
 $TE = \left(\frac{h^2}{3}\right) \left[\frac{\alpha}{\gamma} + \frac{\beta c}{2} - \frac{c^2}{6}\right] (\phi_i^{n+1})_{txx}$
 $+ \left(\frac{h^3}{3}\right) \left[\frac{c^2}{3\gamma} - \frac{c^3}{12} - \frac{1}{6\gamma} - \frac{\alpha}{12} + \frac{\alpha c}{2\gamma} + \frac{\alpha c^3}{12} + \frac{\alpha}{\gamma^2} + \frac{\beta c^2}{4}\right] (\phi_i^{n+1})_{txx} + HOT$
Choosing β to eliminate ϕ_{txx} we have $\beta = \frac{c}{3} - \frac{2\alpha}{\gamma c}$.
Notice that α is only a function of γ , while β depends on γ and α .
 β as a function of α is shown below for several values of c .
The resulting algorithm is third order in space and second order
in time. We will show through examples that it has excellent
amplitude and phase conservation properties. 22



4) As
$$\gamma \to 0$$
, β becomes undefined because $\beta = \frac{c}{3} - \frac{2\alpha}{\gamma c}$. Physically
we must have $u \to 0$, then the difference equation
$$\frac{1}{9\Delta t} \Big[\left(\phi_{i-1}^{n+1} - \phi_{i-1}^{n} \right) + 4 \left(\phi_{i}^{n+1} - \phi_{i}^{n} \right) + \left(\phi_{i+1}^{n+1} - \phi_{i+1}^{n} \right) \Big] \\ - \frac{\alpha}{6\Delta t} \Big[\left(\phi_{i+1}^{n+1} - \phi_{i+1}^{n} \right) - \left(\phi_{i-1}^{n+1} - \phi_{i-1}^{n} \right) \Big] + \frac{u}{6h} \Big[\left(\phi_{i+1}^{n+1} + \phi_{i+1}^{n} \right) - \left(\phi_{i-1}^{n+1} + \phi_{i-1}^{n} \right) \Big] \\ - \Big[\frac{u}{6h} (\alpha - \beta) + \frac{D}{3h^2} \Big] \Big[\left(\phi_{i+1}^{n+1} - 2\phi_{i}^{n+1} + \phi_{i-1}^{n+1} \right) \\ - \Big[\frac{u}{6h} (\alpha + \beta) + \frac{D}{3h^2} \Big] \Big] \Big[\left(\phi_{i+1}^{n+1} - 2\phi_{i}^{n} + \phi_{i-1}^{n} \right) = 0 \Big]$$

becomes independent of β and the algorithm reduces to the Crank-Nicolson-Galerkin method.
5) If $\gamma \to \infty$ then $\alpha \to 1$ and $\beta \to c/3$. This is the purely convective case. The difference equation becomes

24

$$\frac{1}{18\Delta t} \Big[5\Big(\phi_{i-1}^{n+1} - \phi_{i-1}^{n}\Big) + 8\Big(\phi_{i}^{n+1} - \phi_{i}^{n}\Big) - \Big(\phi_{i+1}^{n+1} - \phi_{i+1}^{n}\Big) \Big] \\ + \frac{u}{3h} \Big[\phi_{i}^{n+1} - \phi_{i-1}^{n+1} + \frac{\Delta t}{6h}\Big(\phi_{i+1}^{n+1} - 2\phi_{i}^{n+1} + \phi_{i-1}^{n+1}\Big) \\ + \phi_{i}^{n} - \phi_{i-1}^{n} - \frac{\Delta t}{6h}\Big(\phi_{i+1}^{n} - 2\phi_{i}^{n} + \phi_{i-1}^{n}\Big) \Big] = 0$$

and the truncation error is
$$TE = \frac{h^{3}}{36}(c^{2} - 1)(\phi_{i}^{n+1})_{txxx} + HOT$$

This algorithm is 3d order accurate. If c = 1 the leading term vanishes and the method is super convergent. If β = 0 we go back to a second order scheme.

 Many more Petrov-Galerkin and other methods have been proposed for the transient case. A *BEST* scheme DOES NOT EXIST.











The order of convergence predicted for equation (PG) by the				
truncation eror analysis when $\alpha \neq 0$ and $\beta \neq 0$ is $O(h^3)$.				
To show this, we solve example 2 again, that is				
$\frac{\partial \phi}{\partial t} + 0.25$ but keepi are shown A log-log in the figu	$\frac{\partial \phi}{\partial x} - 0.0003$ ing $c = 0.9$ com in the table of the reare.	$125 \frac{\partial^2 \phi}{\partial x^2} = 0.$ instant. The relative error	0 with 5 different meshes maximum relative errors to $t = 2.07$. vs. the mesh size is shown	
h	Max absolute error	Max relative error	1000	
0.06250	0.149	26.2		
0.05000	0.077	14.0	81	
0.04167	0.046	8.7		
0.025	0.012	2.2	100	
0.00125	0.002	0.3		
			10 31	