A Localized Tau Method P.D.E. Solver

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Introduction

In this paper we present a new form of the collocation method that allows one to find very accurate solutions to time marching problems without the unwelcome appearance of Gibb's phenomenon oscillations. The basic method is applicable to any partial differential equation whose solution is a continuous, albeit possibly rapidly varying function. Discontinuous functions are dealt with by replacing the function in a small neighborhood of the discontinuity with a spline that smoothly connects the function segments on either side of the discontinuity. This will be demonstrated when the solution to the inviscid Burgers equation is discussed.

As is well known it is possible to represent a smooth function with great precision if the representation is made in a basis set of solutions of a singular Sturm-Liouville problem. However if the function varies rapidly unreal oscillations in the representation may occur unless a very large number of terms are used. We consider an alternative approach of dividing the domain of the function into an arbitrary number of subdomains. In each subdomain the function segment will be simple enough to be represented in a low order expansion. Differential equations will be solved separately in each subdomain. Truncation errors inevitably follow from using a finite order expansion and these errors manifest themselves most noticeably as discontinuities across subdomain boundaries in high order derivatives. The tau method will be used to establish continuity of the highest order derivative that occurs in the partial differential equation under consideration. As the function evolves in time the subdomain boundaries will be permitted to move. In this way the growth of instabilities and Gibb's phenomenon ringing will be avoided.

Subdomains

The ideal set of functions to span a finite subregion of a possibly very large domain is the set of Chebyshev polynomials. If a function segment is prescribed in the subdomain $x_{min} \le x \le x_{max}$ of the overall domain $x_b \le x \le x_e$ and the mapping $x' = a_k x + b_k$ such that $x' = -1$ when $x = x_{min}$ and $x' = +1$ when $x = x_{max}$ is performed, then the function at x may be represented by a Chebyshev polynomial expansion at x':

$$f(x) = \sum_{l=0}^{l=N-1} A_l^k T_l(x') \tag{1}$$

The index k identifies the particular subdomain in which x is found. We evaluate the function at the collocation points:

$$x_i' = \cos\left(\frac{i_t \pi}{N-1}\right) \tag{2}$$

where $i_t = -i + N$, and $1 \le i \le N$, with this numbering scheme $x_1' = -1$ and $x_N' = 1$. Then

$$f\left(\frac{x_i' - b_k}{a_k}\right) = \sum_{l=0}^{l=N-1} A_l^k T_l(x_i') \tag{3}$$

or in matrix form:

$$\sum T_{il} A_l^k = f_i^k \tag{4}$$

if N is small the expansion coefficients may be found quickly and accurately by matrix techniques (either inversion or LU decomposition)

If the function segment is well represented by N polynomials then the highest order polynomials should be associated with very small coefficients. Using a simple algorithm discussed below a set of contiguous subdomains can always be found in which the last four expansion coefficients are very small:

$$A^k_{N-3} < \varepsilon, \quad A^k_{N-2} < \varepsilon, \quad A^k_{N-1} < \varepsilon, \quad A^k_N < \varepsilon, \quad \varepsilon << 1$$

In Figure 1 is a superposition of the function $y = e^{-x^2}$ and a Chebyshev representation made in three subdomains with eighteen polynomials in each subdomain:

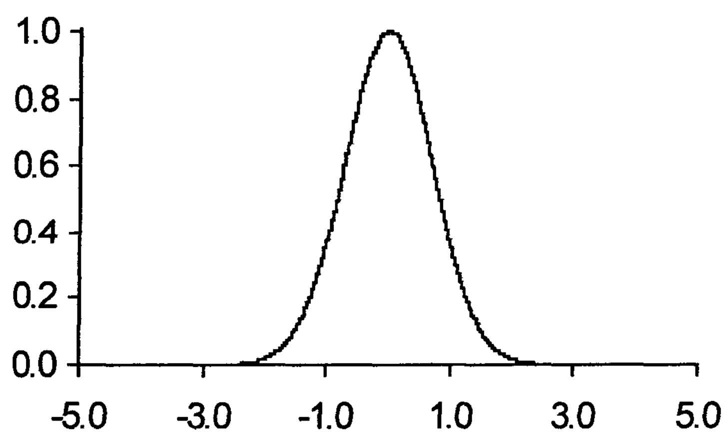

Figure 1: A superposition of a Gaussian and its Chebyshev representation. The curves are virtually indistinguishable

Figures (2)-(4) show each subdomain separately.

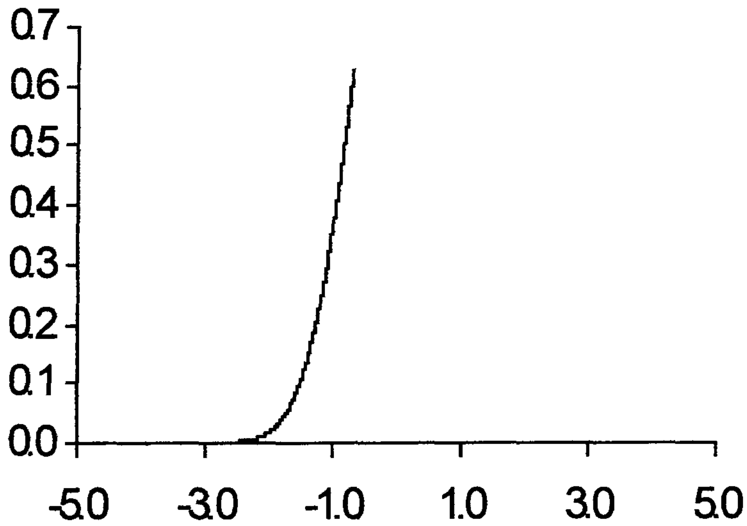

Figure 2. The Chebyshev representation in the first subdomain

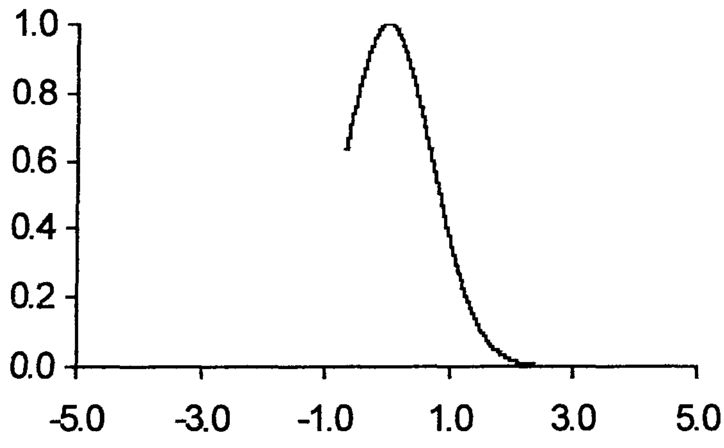

Figure 3. The Chebyshev representation in the second subdomain

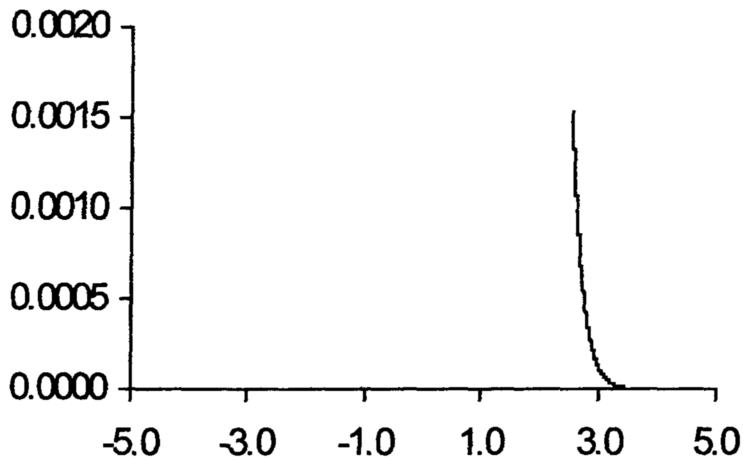

Figure 4. The Chebyshev representation in the third subdomain

Figures (5) and (6) demonstrate the considerable accuracy possible with this method. Figure (5) is a superposition of the nearly singular function:

$$y(x) = \frac{-2\sinh(x)}{\cosh(x) - e^{-.0001}} \tag{5}$$

and its Chebyshev representation. Figure (6) is a superposition of the second derivative of the function and the second derivative of its Chebyshev representation:

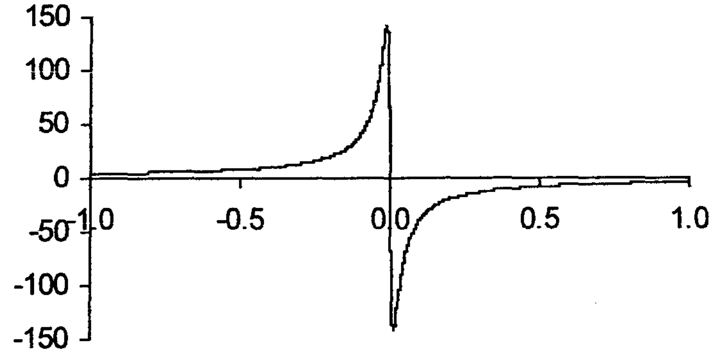

Figure 5. A nearly singular function and its Chebyshev representation

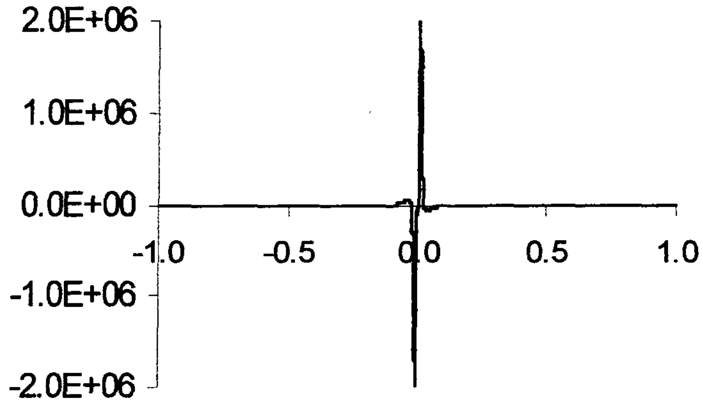

Figure 6. A superposition of the second derivative of the function and the second derivative of its Chebyshev representation The representation of the function and of its rapidly varying second derivative is excellent and there is no sign of Gibb's oscillations.

To form a strategy for finding subdomain boundaries we consider the problem of solving the Burgers equation

$$\frac{\partial y(x,t)}{\partial t} = -y(x,t)\frac{\partial y(x,t)}{\partial x} + \frac{\partial^2 y(x,t)}{\partial x^2} \qquad (6)$$

$y(x,t_0)$ is the function shown in figure (5). Again the function will be treated as a set of function segments in contiguous subdomains each represented by a low order Chebyshev polynomial expansion. We will use the tau method to find expansion coefficients in each subdomain. The tau method adds to the N order expansion m additional terms of order N+1 to N+m, which impose m boundary conditions on the polynomial representation, and it will be used to ameliorate the effects of the most serious source of error, which is the truncation error that occurs in a low order polynomial expansion. The tau method will be used to enforce continuity of the highest order derivative that occurs in the partial differential equation across subdomain boundaries.

Assume that the subdomain labeled k begins at x_a and ends at x_b. In this subdomain x is mapped into x' so that $-1 \le x' \le 1$, and $x' \equiv a_k x + b_k$.
We consider a tau method expansion defined by:

$$\sum_{l=0}^{l=N+1} A_l T_l(x_i') = f(x_i), \quad 1 \le i \le N, \qquad (7)$$

and

$$a_k^2 \sum_{l=0}^{l=N+1} A_l T_l''(-1) = f''(x_a) \qquad (7a)$$

$$a_k^2 \sum_{l=0}^{l=N+1} A_l T_l''(+1) = f''(x_b) \qquad (7b)$$

(note that $\frac{\partial^2}{\partial x^2} = \frac{\partial}{\partial x'^2}\left(\frac{\partial x'}{\partial x}\right)^2 = a_k^2 \frac{\partial}{\partial x'^2}$).

Eqs. (7) form a set of N+2 equations that produce a set of expansion coefficients which represent the function exactly at N collocation points and correctly reproduce the second derivative of the function at the endpoints of the subdomain.

These equations may be combined into the single matrix equation:

$$\sum S_{il} A_l = h_i \tag{8}$$
$$S_{il} \equiv T_l(x'_i), \quad 1 \le i \le N, \ \ 0 \le l \le N+1 \tag{8a}$$
$$S_{N+1l} \equiv T_l''(-1), \quad 0 \le l \le N+1 \tag{8b}$$
$$S_{N+2l} \equiv T_l''(+1), \quad 0 \le l \le N+1 \tag{8c}$$

and

$$h_i = y\left(\frac{x'_i - b_k}{a_k}\right) \qquad 1 \le i \le N \tag{8d}$$
$$h_{N+1} = \frac{y''(x_a)}{a_k^2} \tag{8e}$$
$$h_{N+2} = \frac{y''(x_b)}{a_k^2} \tag{8f}$$

At the inner boundary of the innermost subdomain and at the outer boundary of the outermost subdomain second derivatives need not be specified because there are no neighboring subdomains to match boundary derivatives there. Accordingly for the first subdomain we consider a set of matrices similar to those in eqs. (8) except that the value of the second derivative is needed only at the outer edge:

$$\sum X_{il} A_l = h_i \tag{9}$$

where

$$X_{il} \equiv T_l(x_i^{'}), \quad 1 \le i \le N, \; 0 \le l \le N \tag{9a}$$

$$X_{N+1l} \equiv T_l^{''}(+1), \quad 0 \le l \le N \tag{9b}$$

and

$$h_i = y\left(\frac{x'_i - b_k}{a_k}\right), \qquad 1 \le i \le N \tag{9c}$$

$$h_{N+1} = \frac{y^{''}(x_b)}{a_k^2}, \tag{9d}$$

Solving eqs. (9) for the A_l produces a set of N+1 coefficients $0 \le l \le N$, that exactly reproduce the function at N collocation points, and the correct second derivative at the outer boundary of the innermost subdomain. We include the definition:

$$A_{N+1} \equiv 0 \tag{9e}$$

to create a set of N+2 coefficients as in eqs.(8).

Similarly for the last subdomain:

$$\sum Y_{il} A_l = h_i \tag{10}$$

where

$$Y_{il} \equiv T_l(x_i^{'}), \quad 1 \le i \le N, \; 0 \le l \le N, \tag{10a}$$

$$Y_{N+1l} \equiv T_l''(-1), \quad 0 \le l \le N, \tag{10b}$$

and

$$h_i = y\left(\frac{x'_i - b_k}{a_k}\right), \qquad 1 \le i \le N \tag{10c}$$

$$h_{N+1} = \frac{y''(x_a)}{a_k^2}, \tag{10d}$$

$$A_{N+1} \equiv 0 \tag{10e}$$

Finally there exists the possibility that one subdomain is sufficient in which case the subdomain is identical with the complete computational domain and no boundary matching needs to be done. Then

$$\sum T_{il} A_l = h_i \tag{11}$$

where

$$h_i = y\left(\frac{x'_i - b_k}{a_k}\right), \qquad 1 \le i \le N \tag{11a}$$

Subdomain Boundaries

If the domain of y(x) is $x_a \le x \le x_b$ then let $x_i \equiv x_a$ and $x_f \equiv x_b$ and test the possibility that one subdomain is sufficient. To do this simply map the domain into that appropriate for Chebyshev polynomials: $x_a \to -1, x_b \to +1$, evaluate y(x) at the collocation points, and invert equation (11):

$$A_l^k = \sum_i Z_{li}^{-1} y_i^k \quad \text{for } 1 \le i \le N, \text{ and } 0 \le l \le N-1 \tag{12}$$

to find the Chebyshev coefficients and we define

$$A_N^k \equiv 0, \;\; A_{N+1}^k \equiv 0, \qquad (12a)$$

to create a set of N+2 coefficients. If the representation is a good one then the coefficients of the highest order polynomials will be very small. We apply a test to these high order coefficients:

(1.) Let $A_{\max} \equiv 1$, then.
Find the coefficient whose magnitude, $|A_j|$ is largest. If this quantity is larger than $A_{\max}$ then let $A_{\max} \equiv |A_j|$.

(2.) Compare the highest order coefficients with $A_{\max}$. They must satisfy the smallness test:

$$\left|\frac{A_m^k}{A_{\max}^k}\right| < \varepsilon, \; N-4 \le m \le N+1 \;, \; \varepsilon << 1 \;, \qquad (13)$$

If the smallness test is passed then one subdomain is enough.

Otherwise with $x_i = x_a$ and $x_f = x_b$:
(1.) Let $x_i \equiv x_i$, and redefine x_f so that

$$x_f = c_1 x_i + c_2 x_f \text{ where } c_1 + c_2 = 1. \qquad (14)$$

Then use eqs.(9) (This set of equations is used because x_i is the innermost point in the computational domain), to find the N+2 expansion coefficients and again apply the smallness test. If the test is failed then repeat (1.) until it is passed. This is the innermost subdomain extending from $x_i^{1i} = x_i$ to $x_f^{1i} = x_f$. Then:

(2.) Let $x_i = x_f^{1i}$ and $x_f = x_b$. Use eqs. (10) to find the expansion coefficients (This set of equations is used because x_f is the outermost point in the computational domain), and apply the smallness test. If it is passed then two subdomains are sufficient. Otherwise:

(3.) Let $x_f = x_b$ and

$$x_i = c_2 x_i + c_1 x_f \qquad (15)$$

Use eqs. (10) to find the expansion coefficients and again apply the smallness test. If the test is failed then repeat step (3.) until a sufficiently small subdomain is found. This is the outermost subdomain extending from $x_i^{1o} = x_i$ to $x_f^{1o} = x_b$.

(4.) Return to the inner boundary. Let $x_i = x_f^{1i}$ and $x_f = x_i^{1o}$. Use eqs. (8) to find the expansion coefficients and apply the smallness test. If the test is passed then three subdomains are sufficient. If not then:

(5.) Let $x_i = x_i$ and $x_f = c_1 x_i + c_2 x_f$. Use eqs. (8) to find the expansion coefficients, and apply the smallness test. If the expansion coefficients fail this test then repeat step (5.) until a sufficiently small subdomain is found. This is the second innermost subdomain. It extends from $x_i^{2i} = x_f^{1i}$ to $x_f^{2i} = x_f$.

(6.) Return to the outer boundary. Let $x_i = x_f^{2i}$ and $x_f = x_i^{1o}$ Use eqs. (8) to find the expansion coefficients and apply the smallness test. If the expansion coefficients pass this test then four subdomains are sufficient. If not then:

(7.) Let $x_f = x_i^{1o}$ and $x_i = c_2 x_i + c_1 x_f$. Use eqs. (8) to find the expansion coefficients and again apply the smallness test. If it is failed then repeat step (7.) until a sufficiently small subdomain is found. This is the second outermost subdomain extending from $x_i^{2o} = x_i$ to $x_f^{2o} = x_i^{1o}$.

(8.) Repeat this search pattern, (i.e. next find x_i^{3i} and x_f^{3i}, and then x_i^{3o} and x_f^{3o}, etc.),until a complete set of subdomains is found.

Partial Differential Equations

The solution of the partial differential equation in each subdomain is found through integration over a small time interval followed by a corrector step to match derivatives at subdomain boundaries.

Returning to the Burgers equation as illustration, we see that the right hand side of eq. (6) is:

$$y_i^k(t) = \sum_{l=0}^{l=N+1} T_{il} A_l^k(t) \tag{16}$$

$$y_i^{'k}(t) = a_k \sum_{l=0}^{l=N+1} T_{il}^{'} A_l^k(t) \tag{17}$$

$$y_i^{''k}(t) = a_k^2 \sum_{l=0}^{l=N+1} T_{il}^{''} A_l^k(t) \tag{18}$$

in each subdomain.

Ignoring boundary conditions for the moment; the differential equation in each subdomain becomes

$$\sum T_{il} \frac{dA_l^k(t)}{dt} = -y_i^k(t) y_i^{'k}(t) + y_i^{''k}(t) \equiv g_i^k(t) \tag{19}$$

Boundary equations are established by specifying g_1^1, g_N^{last} and by averaging the P.D.E. operator at the outer boundary of one subdomain and the inner boundary of the neighboring subdomain.

$$g_N^{k-1}(t) \equiv \frac{-y_N^{k-1}(t)y_N^{'k-1}(t) + y_N^{''k-1}(t) - y_1^k(t)y(t)_1^{'k} + y_1^{''k}(t)}{2} \tag{20}$$

$$g_1^k(t) \equiv g_N^{k-1}(t) \tag{21}$$

then

$$\frac{dA_l^k(t)}{dt} = T_{li}^{-1} g_i^k(t) \tag{22}$$

is an ordinary differential equation for N expansion coefficients which may be solved using standard methods such as Runge-Kutta integration. The solutions to eq. (22) will maintain continuity of the function across subdomain boundaries but the derivatives are unconstrained and can become noticeably discontinuous. To impose continuity of the highest order derivative that occurs in the P.D.E. at subdomain boundaries we invoke the following corrector:

We begin with eqn (22) which provides an initial expression for $\frac{dA_l^k(t)}{dt}$, and this is used to calculate $\frac{dy_i^k(t)}{dt}$ at each collocation point:

$$\frac{dy_i^k(t)}{dt} = \sum T_{il} \frac{dA_l^k(t)}{dt} \tag{23}$$

and the change in time of the highest order derivative at each boundary point:

$$\frac{dy_N^{n,k}}{dt} = a_k^n \sum T_{Nl}^n \frac{dA_l^k(t)}{dt} \tag{24}$$

$$\frac{dy_1^{n,k}}{dt} = a_k^n \sum T_{1l}^n \frac{dA_l^k(t)}{dt} \tag{25}$$

$\frac{dy_1^{n,k}}{dt}$ and $\frac{dy_N^{n,k-1}}{dt}$ are the same quantities evaluated at the common boundary of neighboring subdomains. To enforce equality the corrector step replaces these quantities by their averages:

$$\frac{dy^{n,k}}{dt} \equiv \frac{\frac{dy_1^{n,k}}{dt} + \frac{dy_N^{n,k-1}}{dt}}{2} \tag{26}$$

$$\frac{dy_1^{n,k}}{dt} \equiv \frac{dy^{n,k}}{dt} \tag{27}$$

$$\frac{dy_N^{n,k-1}}{dt} \equiv \frac{dy^{n,k}}{dt} \tag{28}$$

and uses these averages in matrix operations similar to those defined by eqs. (8). For example in an interior subdomain we have

$$\sum_l S_{il} \frac{dA_l^k}{dt} = h_i^k \tag{29}$$

where

$$h_i^k = \frac{dy_i^k(t)}{dt}, \qquad 1 \le i \le N \tag{30}$$

$$h_{N+1}^k = \frac{dy_1^{n,k}(t)}{dt} \cdot \frac{1}{a_k^n} \tag{31}$$

$$h_{N+2}^k = \frac{dy_N^{n,k}(t)}{dt} \cdot \frac{1}{a_k^n} \tag{32}$$

Then

$$\frac{dA_l^k(t)}{dt} = \sum_{i=1}^{N+2} S_{li}^{-1} h_i^k(t) , \qquad 0 \le l \le N+1 \qquad (33)$$

is an ordinary differential equation for the rate of change of the expansion coefficients which maintains continuity of the function and its highest order derivative at the common boundary of subdomain k and subdomain k+1, and at the common boundary of subdomain k and k-1.

Moving Boundaries

Repeated integration of equation (33) results in the growth of discontinuities in high order derivatives at subdomain boundaries. To stop the growth of these discontinuities it is necessary to halt the process from time to time and find a new set of subdomains whose boundaries are different from those of the present set. There is no unique rule for determining when this should be done, but one effective rule follows from monitoring the growth of the high order polynomial coefficients. If originally the function in each subdomain is described by the polynomial coefficients $A_l^{original}$ the high order terms are defined to be those for which $\left|\frac{A_l^{original}}{A_{\max}^{original}}\right| < \varepsilon$ for all $l > L$. As time goes on we test for the condition

$$\left|A_l\right| - \left|A_l^{original}\right| > \varepsilon \qquad \text{for } l > L \qquad (34)$$

When this condition is met the high order terms are growing and new boundaries must be found. To do this, simply stop the integration routine, treat the present state as the initial condition and reapply the algorithm for finding subdomains discussed above except that a search from $x_{initial}$ to x_{final} should alternate with a search from x_{final} to $x_{initial}$.

In summary solving P.D.E.'s using this localized collocation method is a three-step process:

(1.) Find a set of subdomains in which a function is represented by a small set of Chebyshev polynomials.

(2) Solve the O.D.E. eqn (33) in each subdomain.

(3) Test for the growth of high order coefficients with eqn (34). If eqn (34) is satisfied then reinitialize the problem by returning to step (1).

Examples

The solution to Burgers equation without boundary conditions and with

$y(x,t_0=.0001)=\dfrac{-2\sinh(x)}{\cosh(x)-e^{-.0001}}$ as the initial state is:

$$y(x,t)=\frac{-2\sinh(x)}{\cosh(x)-e^{-t}} \qquad (35)$$

A superposition of numerical and analytic solutions at various times is plotted in figure (7). The numerical solution has the boundary conditions that $y(-1,t)$ and $y(1,t)$ are constant in time The numerical solution is indistinguishable from the analytic except after a long time when the difference in boundary conditions becomes important. This is shown in figure 8.

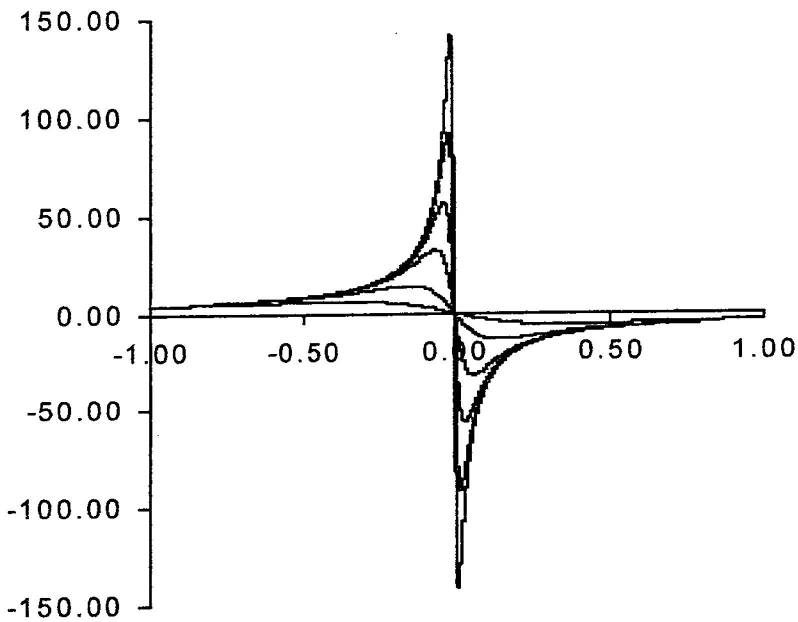

Figure 7 Solution to Burgers Equation. Each curve is a superposition of numerical and analytic solutions.

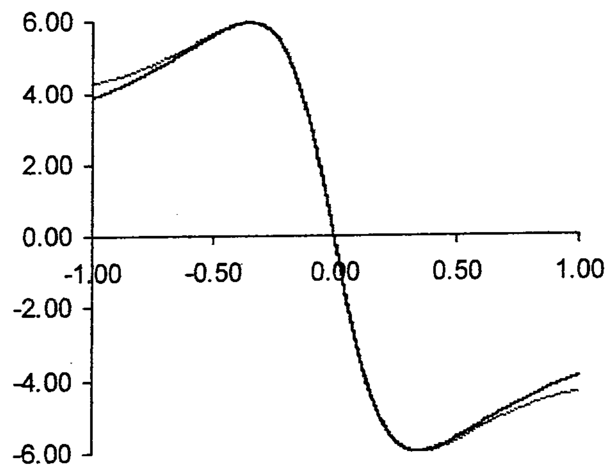

Figure 8 Boundary Effects. The thick line is the analytic solution with no boundary conditions, the thin line is the numerical solution with no change allowed at the boundaries.

A more interesting example is the Kortweg –Devries equation.

$$\frac{\partial y(x,t)}{\partial t}=\frac{-\partial y(x,t)}{\partial x}(1+y(x,t))+\frac{-\partial^3 y(x,t)}{\partial x^3} \tag{36}$$

As the initial state we use:

$$y\left(x,t\big|_{t=0}\right)=-12\cosh(x)^{-2} \tag{37}$$

This equation has the soliton solution

$$y(x,t)=-12\cosh(x-5t)^{-2} \tag{38}$$

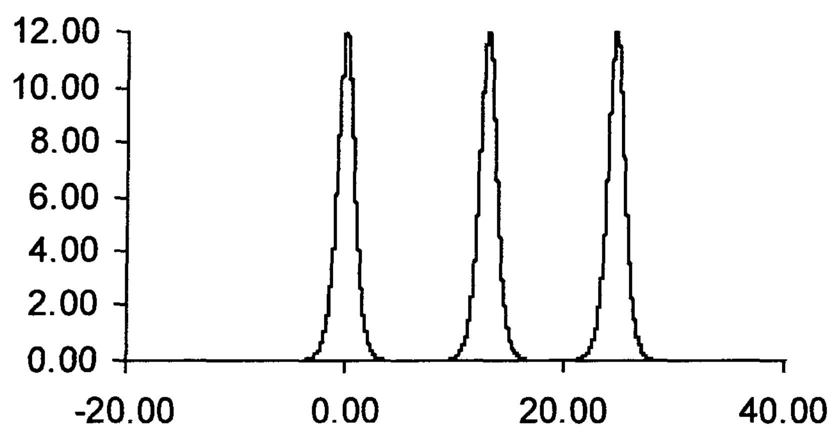

Figure 9 Each curve is a superposition of the numerical and analytic solutions of the Kortweg-deVries equation at different moments in time.

The wave equation is second order in time:

$$\frac{\partial^2 y(x,t)}{\partial t^2} = \frac{\partial^2 y(x,t)}{\partial x^2} \tag{39}$$

with the initial state

$$y(x,t|_{t=0}) = \cos\left(\frac{\pi x}{2}\right)^{100} \tag{40}$$

The figure below shows the solution at different moments in time.

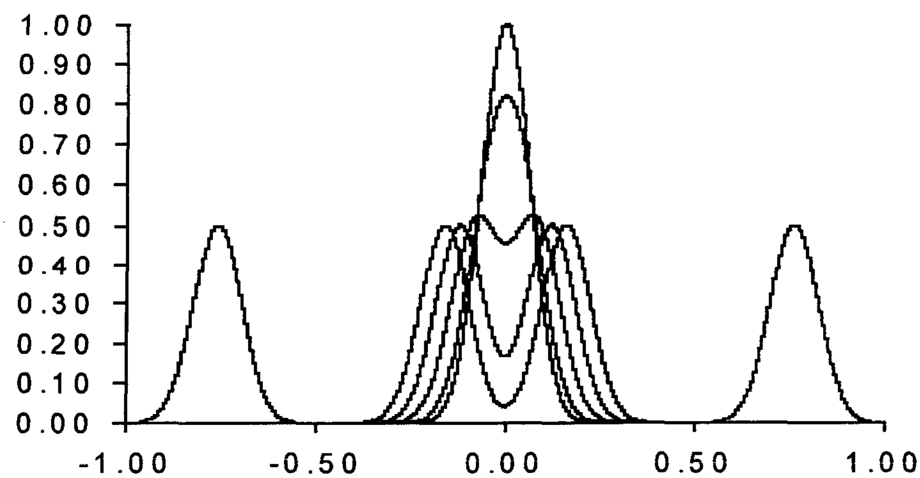

Figure 10. Initial pulse dividing in half and traveling in opposite directions

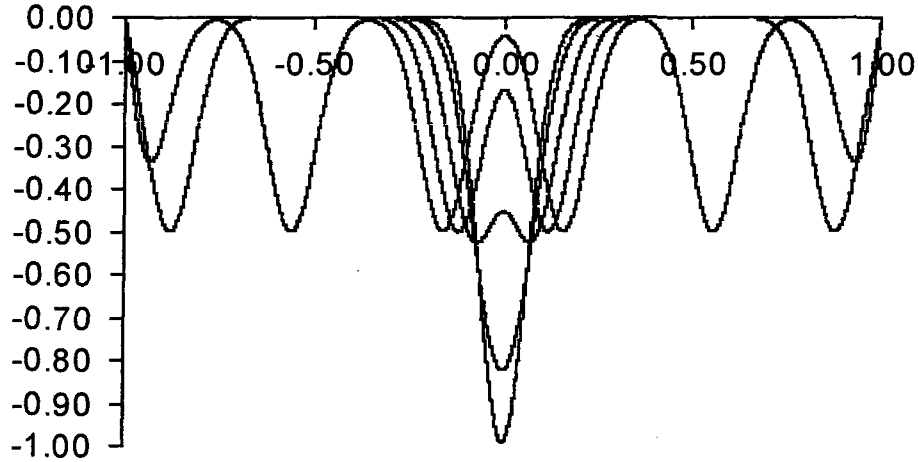

Figure 11 Reflected wave which reassembles at the center

Finally, to demonstrate the effect of the occurrence of a singularity consider the inviscid Burgers equation

$$\frac{\partial y(x,t)}{\partial t} = -y(x,t)\frac{\partial y(x,t)}{\partial x} \tag{42}$$

with

$$y(x,t_0) = \cos(\pi x)^4, \quad -1 \le x \le 1, \tag{43}$$

as the initial state. As the wave becomes steeper the size of the subdomains near the leading edge become smaller. When one falls below an arbitrary threshold in size a singular region is assumed to have been found, and the function in a small neighborhood of the singularity is replaced by a spline. The spline is a sixth order polynomial whose coefficients are determined by the value of the function and its first and second derivatives at the boundaries of the singular region.

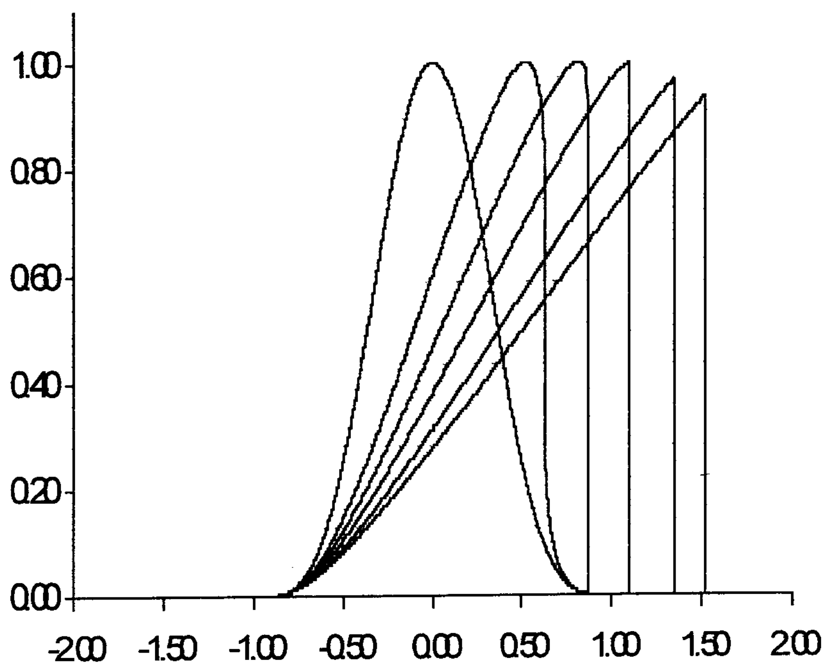

Figure 12 Numerical Solution to the Inviscid Burgers Equation