CHAPTER 14

Adaptive Multi-Domain Spectral Methods[1]

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Abstract

When pseudo-spectral methods are used with domain decomposition procedures i the numerical solution of partial differential equations, the use of multiple domains can significantly effect the accuracy of the approximation. If large gradients occur near the boundaries of the domain then the accuracy can be enhanced, while if the rapid variations occur in the interior of the subdomains then the accuracy can be degraded. We have developed an adaptive multi-domain method. In this method we employ functionals, defined within each sub-domain, which measure the error in the pseudo-spectral approximation. Using polynomial interpolation, these functionals can be evaluated for arbitrary location of the interfaces. The location of the interfaces can then be determined so as to minimize the maximum error in all of the subdomains, or to equalize the errors within the subdomains. We have implemented an adaptive multi-domain pseudo-spectral method for the solution of one-dimensional wave equations. Computed results demonstrate that the use of adaptive multi-domain methods can result in significantly enhanced accuracy for a fixed number of collocation points.

1. Introduction. The accuracy of Chebyshev pseudo-spectral methods in approximating solutions to partial differential equations, can be degraded when used to approximate solutions which have localized regions of rapid variation. Such problems occur in many application areas, for example combustion, fluid dynamics, solid mechanics and wave propagation. The approximations can exhibit spurious oscillations which can lead to nonlinear instabilities. The accuracy is also sensitive to the location of regions of rapid variation. There is significant evidence, for example, that pseudo-spectral methods are more effective in approximating functions where rapid variations or large gradients occur close to the boundary of the region, as opposed to the interior, e.g. [5, 14].

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One approach to improve the accuracy of spectral and pseudo-spectral approximations to rapidly varying functions is to employ mappings which have been determined adaptively to minimize a functional of the solution which measures the error in the approximation [1, 2, 3, 4, 10]. This adaptive procedure has been employed in the study of a variety of problems where the solutions exhibit localized regions of rapid variation, for example in combustion, and has been found to be effective when there is only a single region of rapid variation or when there are multiple regions which are not widely separated.

When there are multiple regions of rapid variation which are widely separated, the effectiveness of many families of mappings degrades. In this case the accuracy of Chebyshev spectral and pseudo-spectral approximations can be improved by employing domain decomposition techniques in which the domain is sub-divided into two or more subdomains. If the subdomains are properly chosen, for example to have each domain include only a single region of rapid variation, accurate approximations can be obtained [5].

However, when pseudo-spectral methods are used with domain decomposition procedures the accuracy of the approximation can be very sensitive to the location of the subdomains. If, for example, the regions of large gradients occur near the boundaries of the subdomains then the accuracy can be enhanced, while if the rapid variations occur in the interior of the subdomains then the accuracy can be degraded.

In many problems the behavior of the solution, in particular the location of regions of rapid variation, can change significantly in time. In these cases the use of multi-domain pseudo-spectral methods, with interfaces which are fixed in time can result in inaccurate approximations, even if the interfaces are chosen initially to provide adequate resolution of the initial data.

In this paper we describe a procedure to determine the location of the interfaces adaptively based on properties of the solution. The procedure utilizes functionals which have been previously employed in single domain adaptive procedures to estimate the error in the pseudo-spectral approximation. In these applications the functionals are used to determine coordinate transformations in which the error is minimized. In this paper the functionals are employed to determine interface locations in which the errors are either minimized or equally distributed among the different subdomains. The adaptive procedure is described in section 2. In section 3 we illustrate the method with computations for a linear system of equations describing wave propagation.

2. Numerical Method. We first describe the standard pseudo-spectral method. This description will be brief, more details can be found in [6, 7, 9]. For concreteness we consider a one-dimensional model equation

$$u_t = u_{xx} + R(u), \quad -1 \le x \le 1, \tag{1}$$

where $R(u)$ represents a nonlinear term not involving derivatives. We assume that the problem has been scaled to the interval I, $\{-1 \le x \le 1\}$. The solution is approximated by expanding u as a finite sum of Chebyshev polynomials

$$u \simeq u_J \equiv \sum_{j=0}^{J} a_j T_j(x). \tag{2}$$

In the pseudo-spectral method the expansion coefficients a_j are obtained from collocation, that is the function u_J is forced to solve (1) at a set of $J+1$ points x_j, called the collocation points. The unknowns of the problem are the values of u_J at the collocation points. Pseudo-spectral methods are particularly well suited to nonlinear problems because the nonlinearities are evaluated directly in terms of function values at the collocation points. The expansion (2) is used only for the purposes of computing spatial derivatives. Typically the collocation points are the Gauss-Lobatto points,

$$x_j = \cos(j\pi/J) \quad (j = 0, \ldots, J).$$

The major advantage of pseudo-spectral methods over finite difference methods is enhanced accuracy for a fixed number of collocation points. In fact pseudo-spectral methods exhibit infinite order accuracy. That is, the error $e = u - u_J$ satisfies, in an appropriate norm,

$$\|e\| = O(J^{-r})$$

for all $r \geq 0$ provided u is sufficiently differentiable. This is in contrast to finite difference methods where the error is of a fixed order, for example $O(J^{-2})$ for a second order method. In practice spectral methods have been shown to be significantly more accurate than finite difference methods for a variety of problems in application areas such as fluid dynamics and meteorology [6, 7, 9].

Pseudo-spectral methods, however, are prone to inaccuracies and oscillations when used to approximate functions with localized regions of rapid variation which occur in many application areas. In addition there is evidence that these methods are significantly more accurate when the region of rapid variation is located close to the boundaries, for example [5, 9, 14]. However even boundary layers can exhibit oscillations if the layers are sufficiently thin.

One approach to enhance the accuracy of pseudo-spectral methods is to employ coordinate transformations so that in the transformed coordinate the function varies more gradually and so can be better approximated by a polynomial expansion. Specifically assume that a family of mappings,

$$x = q(s, \vec{\alpha}), \tag{3}$$

is introduced. Here x represents the physical coordinate, $-1 \leq s \leq 1$ is the transformed coordinate, and $\vec{\alpha}$ denotes one or possibly more free parameters. The pseudo-spectral method can then be applied to the transformed equation to approximate the transformed function $u(q(s, \vec{\alpha}), t)$. The effect of the mapping can be regarded as transforming the function to be approximated to $u(q(s, \vec{\alpha}))$ from $u(x)$. If the mapping is properly chosen $u(q(s, \vec{\alpha}))$ will vary more gradually and so be more readily approximated by a polynomial expansion.

In applications involving the solution of partial differential equations an appropriate coordinate system is generally not known beforehand and must be determined adaptively from the solution. An adaptive procedure was described in [2]. In this procedure a functional which monitors the spectral interpolation error is introduced and the coordinate transformation is chosen so as to minimize the functional. A family of such functionals was derived. One member of this family is

$$I_2(g) = \left(\int_{-1}^{1} (\mathcal{L}^2 g)^2 / w(s) ds \right)^{\frac{1}{2}}, \tag{4}$$

where

$$w(s) = \sqrt{1 - s^2}, \quad \mathcal{L} = w(s) \frac{d}{ds}.$$

If we consider the expansion of a function in terms of Chebyshev polynomials

$$u = \sum_{j=0}^{\infty} a_j T_j(x), \tag{5}$$

where

$$a_j = 2/(\pi c_j) \int_{-1}^{1} u(s) T_j(s) / w(s) ds,$$

and

$$c_0 = 2, c_j = 1, J > 0,$$

then it can be shown [2] that $I_2(g)/j^2$ leads to an upper bound on the size of the coefficients a_j, i.e.

$$| a_j | \leq 2/(\pi c_j) I_2(u)/j^2. \tag{6}$$

It was further shown in [2] that (6) leads to gives an upper bound on the maximum norm of the error in approximating u by either its spectral or pseudo-spectral approximation. Therefore assuming J is given, (4) can be used to estimate the size of the error (alternatively with (4) known and an error level given the number of collocation points, J, can be estimated.

This method is effective in enhancing the accuracy of approximations for solutions with a single region of rapid variation, or for solutions with multiple regions of rapid variation which are not widely spaced. However single domain computations using adaptively chosen coordinate transformations are less effective in approximating functions with multiple regions of rapid variation which are widely spaced, such as a function consisting of several separated spikes [5]. This procedure is less effective because the mapping families depending on a small number of parameters can not generally increase resolution in widely separated spatial regions. In such cases a possible approach is to employ multiple domains.

We first describe a spectral multiple domain method. In such a method the interval I is divided into one or more subintervals and the problem solved in each subinterval with appropriate interface conditions connecting the solution across the subdomain boundaries. At the interface points, appropriate interface conditions are imposed, for example continuity of u and u_x for problems involving two spatial derivatives or characteristic conditions for hyperbolic problems. Discussions of appropriate interface conditions can be found in [7, 8, 12, 13]. In the applications described in Section 3, we solve a linear hyperbolic problem and each characteristic variable is taken from the appropriate subdomain, depending on the propagation direction.

Multiple domain approaches offer several advantages. One major advantage is the possibility of parallel computation in which the computations associated with the different subdomains can be partitioned among different processors. In addition they often allow better conditioned matrices and larger timesteps than single domain calculations. Another important effect of multiple domain approaches is that they can significantly enhance (or degrade) the accuracy of the approximation.

The use of multiple domains can lead to an improvement in accuracy by (a) resolving small scale structures in the problem by introducing domains corresponding to the length scales appropriate of the small scale structures (b) choosing the interface so that the small scale structures or rapid variations occur near the boundary, and (c) isolating different regions of rapid variations within each subdomain and then employing mappings within each subdomain as described above. These properties depend on the choice of the subdomains and a poor choice can lead to a significant degradation in accuracy. In this paper we describe adaptive procedures to determine the location of the interfaces based on properties of the solution and the functional (4). The principles are based on either minimizing the maximum error within each subdomain or equalizing the error within the different subdomains. The methods are described here, more details can be found in [11].

We consider, for simplicity only, the case with two subdomains with interface point Q, although the methods have been implemented using more than two subdomains. Assume that we nave N_1 points in the first subdomain and N_2 points in the second subdomain. If w is a function to be approximated then we denote by w^1, w^2, the function w restricted to each subdomain. Each subdomain can be mapped into the interval I by a simple linear mapping. We can therefore consider w^1 and w^2 as functions of s where $-1 \leq s \leq 1$. Within each subdomain we can then construct the functionals (4) to monitor the error in the subdomain, i.e. $I_2(w^1)/N_1^2$, $I_2(w^1)/N_2^2$. We note that these quantities depend on both w and Q.

Generally there are many parameters to consider in an adaptive domain decomposition procedure. In addition to the locations of the interfaces, the number of domains must be determined and the number of points within each subdomain. In this paper we consider the case where there is an equal number of points in each subdomain. This restriction is generally preferable for parallel processing as the load can be equally balanced among the different processors.

The computational resources will generally be used most efficiently if the errors within the two domains are comparable. The errors within each subdomain can be equalized by determining Q so that

$$| I_2(w^1) - I_2(w^2) | \tag{7}$$

is minimized. We note that if the function w is given the value of (7) is a function only of Q. An alternative formulation is to minimize the largest error within the different subdomains. This strategy can be implemented by choosing Q so that the maximum of $I_2(w^1)$, $I_2(w^2)$ is minimized. This approach can also lead to a significant improvement in the accuracy of the approximation although we have found that equalizing the errors tends to be somewhat more flexible and robust, particularly when there are more than two subdomains. In the remainder of this paper we will concentrate on the implementation of (7) to adaptively determine the location of the subdomains.

3. Results. We consider the hyperbolic system

$$u_t = v_x, v_t = C^2 u_x, -1 \leq x \leq 1. \tag{8}$$

This system models the propagation of one dimensional waves with speed $C(x)$. If C is constant the waves travel with constant shape, i.e. the wave propagation is non-dispersive, while if C is non-constant the propagation is dispersive. At the boundaries $x = \pm 1$ we impose the boundary conditions

$$v + C(1)u = 0, x = 1,$$
$$v - C(1)u = 0, x = -1.$$

These boundary conditions assume that the data corresponding to characteristics entering the region from the exterior is zero. Both u and v are specified as Gaussians at $t = 0$. The precise relationship between u and v depends on whether we want the solution to describe only a single pulse propagating in one direction or two pulses propagating in different directions. In the first case we impose

$$u = v = g(x), g(x) = \exp(-\sigma^2 x^2/2),$$

while in the second case u and v are different multiples of $g(x)$. We have obtained results for $\sigma = 50$ and for $\sigma = 100$.

The system (8) is solved using a Chebyshev pseudo-spectral multi-domain method. We assume an equal number of points in each subdomain. The equations are updated in time using a three stage, low storage Runge-Kutta scheme. At the domain interfaces, the solution is patched using characteristic variables from the appropriate domain [12].

The locations of the interfaces are varied dynamically during the calculations in order to equalize the error, as measured by the functional (4), in each sub-domain. We describe some details of the implementation. Further details can be found in [11]. Consider first the case where there are two subdomains with an interface point $x = Q$. Each subdomain is mapped to the interval $-1 \leq s \leq 1$ using a linear mapping. Letting w denote some specified combination of u and v, we can compute $I_2(w^1)$ and $I_2(w^2)$ At selected intervals of time, we search for a new interface. The interface is determined so that

$$| I_2(w^1) - I_2(w^2) |$$

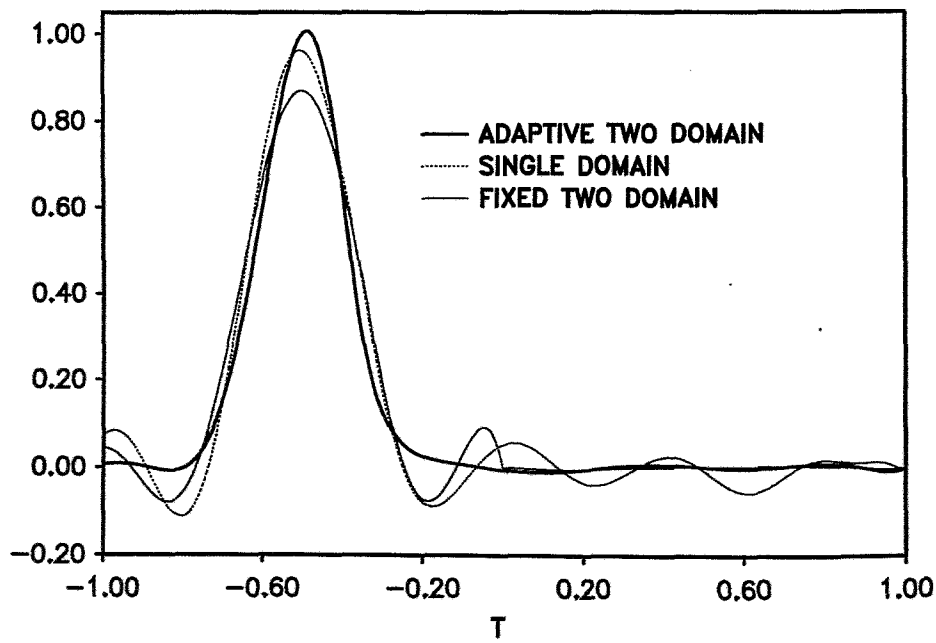
is minimized. This is done as follows. Consider a trial value for the interface point $\tilde{Q}$. The solution w can be interpolated to the collocation points in the subdomains determined by $\tilde{Q}$ using the global Chebyshev expansion for w. We denote the interpolated functions as $\tilde{w}^1$ and $\tilde{w}^2$. We then compute

$$| I_2(\tilde{w}^1) - I_2(\tilde{w}^2) | . \tag{9}$$

Thus (9) can be computed for any value $\tilde{Q}$. We then employ a bisection method to minimize (9). Generally we have found that only a crude minimization is necessary in order to obtain significant improvements over single domain and fixed multi-domain calculations.

We have also implemented this method with three subdomains. In this case we have two interface points Q_1, Q_2. The new values of the interface points are obtained by proceeding from left to right. That is we first hold Q_2 fixed and obtain a minimum by varying Q_1 and attempting to equalize the values of (4) within the subdomains on either side of Q_1. We then hold the new value of Q_1 fixed and find a new value of Q_2.

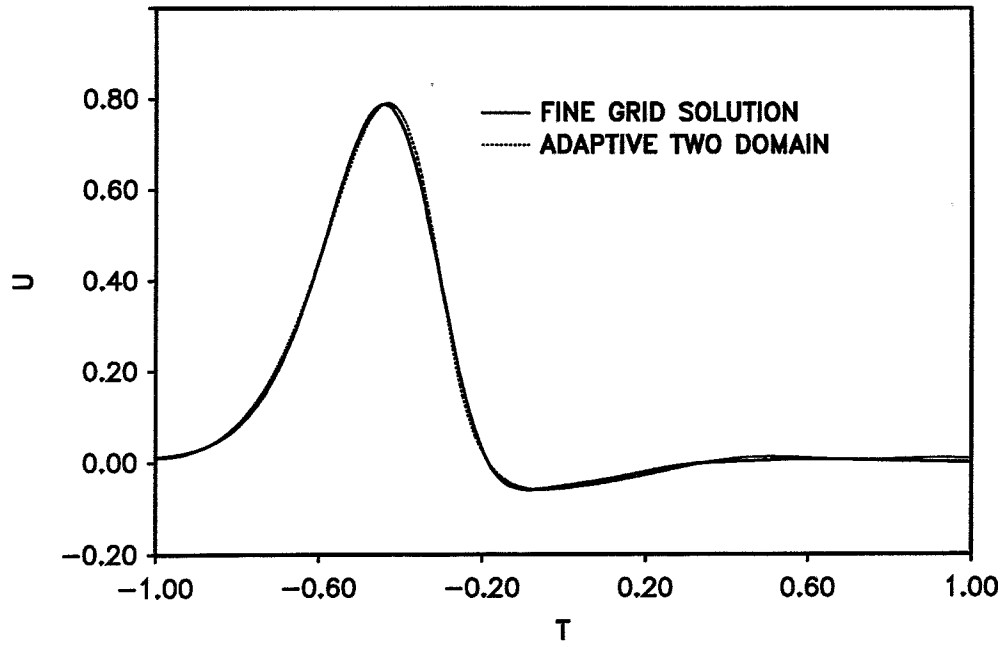
We first illustrate the method for the case of a single Gaussian pulse initially centered at $x = 0$ and propagating to the left. In this case we set $C(x) = 1$ so that the pulse should propagate without distortion. We used two subdomains. In Figure 1 we plot $u(x, t = 0.5)$ for the adaptive two domain calculation with 9 points in each subdomain, a two domain calculation with the interface fixed at $x = 0$ and 9 points in each subdomain, and a single domain calculation with 17 collocation points. In view of the coarse grids, we have interpolated the solution to a fine grid for plotting purposes using the Chebyshev interpolant. This was done in all of the graphs presented in this paper. The reduction in numerical dispersion with the adaptive multi-domain procedure can be clearly seen from the figure.



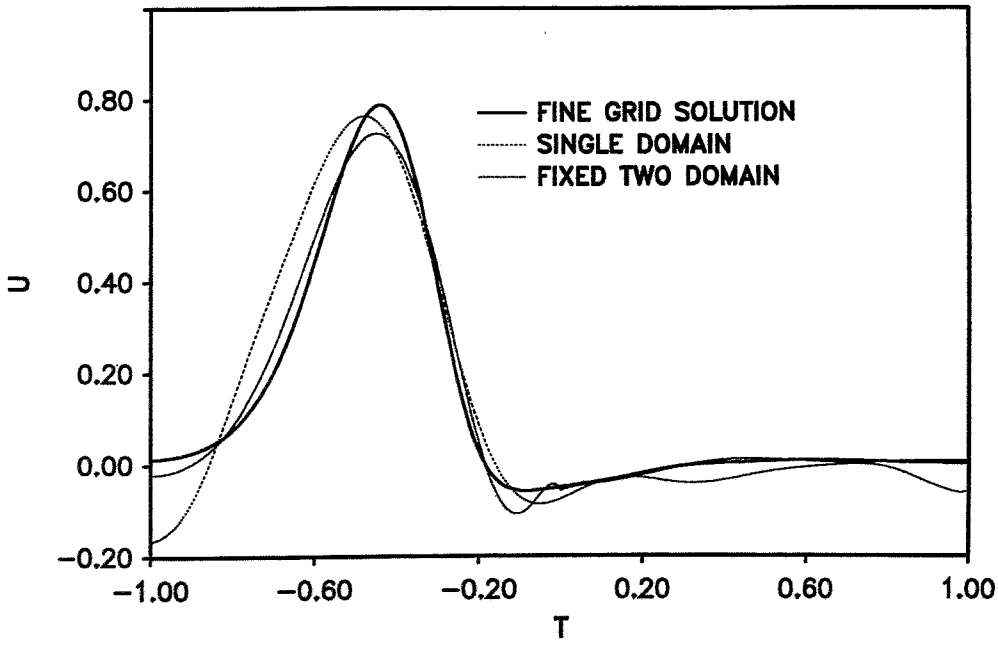
1. Single pulse with $C = 1$.

We next illustrate a case with variable propagation velocity. In this case $C(x) = 1+2x^2$. We compare the computed solutions using two domains with a single domain fine grid solution which we take as exact. This solution was obtained using 65 collocation points. In Figure 2a we plot $u(x, t = 0.4)$ for both the fine grid and the solution obtained using

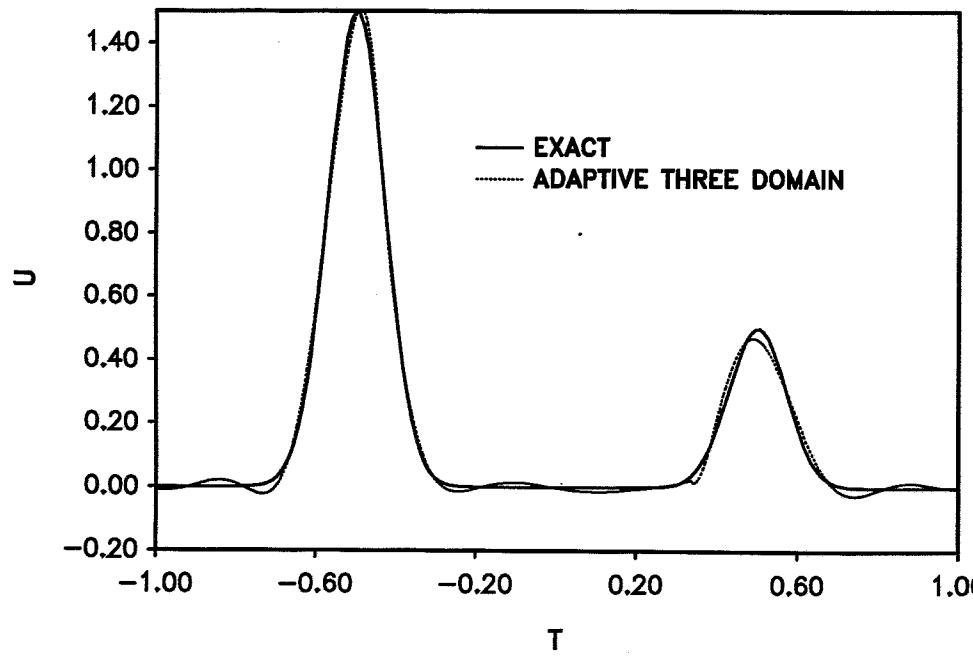
the adaptive multi-domain procedure with 9 points in each subdomain. In Figure 2b we compare the fine grid solution with solutions obtained from a single domain calculation with $N = 17$ and a two domain calculation with the interface fixed at $x = 0$ and with 9 collocation points in each subdomain. The adaptive multi-domain solution is nearly indistinguishable from the fine grid solution while the nonadaptive calculations exhibit noticeable differences.



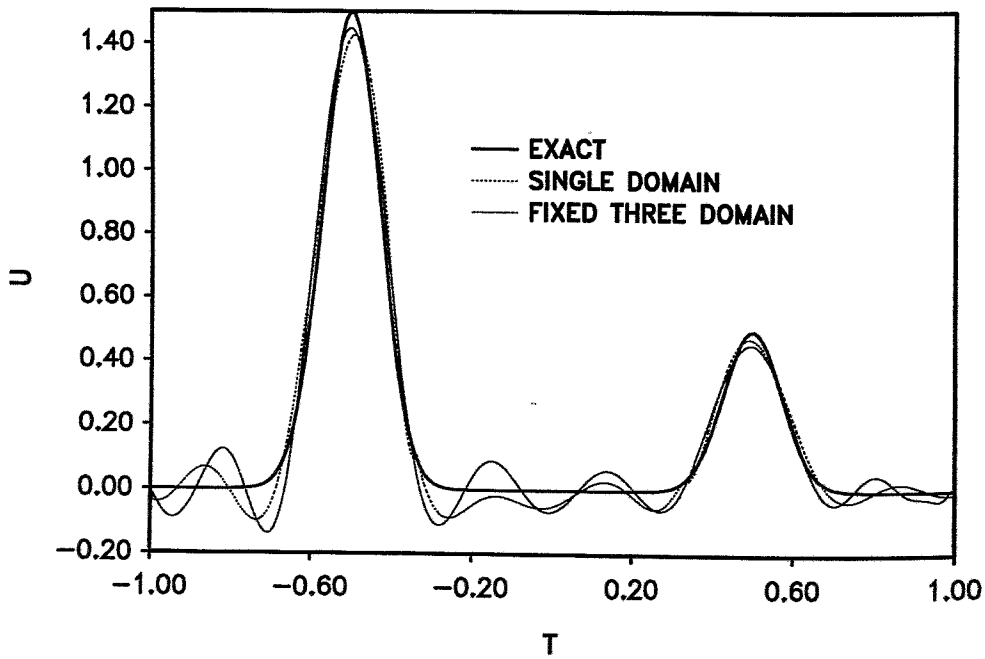
2a. Computation with $C = 1 + x^2$ comparing fine grid solution with adaptive two domain calculation.



2b. Computation with $C = 1 + x^2$ comparing fine grid solution with single domain and fixed two domain calculation.



3a. Two pulse calculation, comparing exact solution with adaptive three domain calculation.



3b. Two pulse calculation, comparing exact solution with single domain calculation and fixed three domain calculation.

As a last example we consider a three domain calculation. In this case $C = 1$ and we set $u = g(x), v = g(x)/2$ at $t = 0$. Thus there are pulses which emanate from $x = 0$ in both directions. We have considered the cases $\sigma = 50$ and $\sigma = 100$. The adaptive procedure improves the accuracy in both cases. We present results for the case $\sigma = 100$. In Figure 3a we compare $u(x, t = 0.5)$ for the fine grid exact solution for u with an adaptive three domain calculation using 9 points in each subdomain. In Figure 3b we plot the exact solution, the results of a single domain calculation with 25 collocation points and a three domain calculation with 9 points in each subdomain and the interfaces fixed at $x = \pm 1/3$. The improvement in accuracy due to the adaptive procedure is evident.

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