CHAPTER 23

Domain Decomposition to Solve Layers and Singular Perturbation Problems*

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Abstract

Our aim concerns the numerical computation of stiff nonlinear PDEs that are appropriate for singular perturbation analysis. We present two domain decomposition methods that numerically solve for the layers of the singular perturbation problem. These numerical methods use at different stages the information given by the asymptotic analysis. We will consider as a test problem the simplified model of reacting flow of Majda [13].

Resumé:

Nous etudions le calcul numerique de problemes raides qui relevent d'une analyse de perturbation singuliere. Nous presentons deux methodes de decomposition de domaine qui resolvent les couches limites du probleme de perturbation singuliere. Ces deux methodes numeriques utilisent a differents niveaux les renseignements obtenus par une analyse asymptotique. Nous considerons comme probleme test le modele de flot reactif simplifie de Majda.

1 Introduction

Our aim concerns the numerical computation of stiff nonlinear PDEs that are relevant in singular perturbation analysis. We present two domain decomposition methods that numerically solve the layers of a singular perturbation problem of the following type

$$-\epsilon\frac{\partial}{\partial x}\left(P(U)\frac{\partial U}{\partial x}\right)+\frac{\partial U}{\partial t}+\frac{\partial}{\partial x}F(U)+\epsilon^{-1}D(U)=0.$$

We show that the combination of asymptotic and numerical analysis provides improved accuracy and/or improved efficiency for such multiple scale problems.

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Many physical problems have multiple scales. A typical situation occurs when physics on the fastest scale induces narrow regions where the variation in the solution is large. Such regions are called *boundary layers* (BL) or *transition layers* (TL) depending on whether they are near a boundary or inside the interior of the domain. These problems are generally relevant for singular perturbation analysis. It seems a natural idea to implement some of the results of this analysis in the numerical computation. The interest in this field of research has been increasing in the last few years (see [1] [5] [6] and their references).

In this paper, we first present an asymptotic induced numerical method based on a hyperbolic scheme. The idea is that the matched asymptotic technique [7] is typically a domain decomposition method. In such asymptotic analysis, one splits the domain into subdomains where different processes occur; one looks for the correct scaling in each subdomain and derives the appropriate subproblems; then one uses the matching relations to connect the subproblems, and so on. The asymptotic induced numerical method that we present is a numerical algorithm that is in some sense the image of the matched asymptotic analysis. Also, the matched asymptotic relations, that are difficult to check analytically, are validated through the computation of the residual. This method has been applied to a singular perturbation problem driven by conservation laws, for example the isentropic gasdynamics equations with a physical viscosity, in [4], [11]; in this paper we extend the method to a model of reacting flows.

Secondly, we present an adaptive domain decomposition method in the context of pseudospectral methods with Chebyshev polynomials. The idea is to use what one knows from the analysis as part of the criteria for the adaptivity. Stiff fronts are a major difficulty in the use of spectral methods. Very efficient adaptive methods have been developed in [3] that solve stiff problems. This method has been extended in [2] to adaptive domain decomposition. We show how one can enhance this adaptive method for singular perturbation problems: the position of the interfaces, the choice of the mapping, the strategy of the domain decomposition can be effectively related to the asymptotic analysis.

We will consider here as a test problem the simplified model of reacting flow of Majda. It has been shown in [13] that this model contains some of the numerical difficulties for reacting flows. This model plays the role of the Burgers' equation for the Navier Stokes equations. In particular, in the computation of reacting shock waves, in this simplified model one can see that the viscosity balances the source terms in the layer and influences the speed of propagation. So one cannot expect to compute such phenomena with a classical hyperbolic scheme. In addition, as shown in [13], a splitting method applied to the operator required an order of magnitude more discretization points than to compute, for example, a Buckley & Leverett equation in the one dimension case. We demonstrate the efficiency of our domain decomposition method for the difficult case of reacting shock layer.

In the interest of brevity, we relegate the details of the asymptotic analysis and more numerical results to the companion paper [10].

2 Asymptotic-induced numerical methods based on a hyperbolic scheme

Let us first briefly recall the ideas of an asymptotic-induced numerical method for a singular perturbation problem driven by a conservation law [9]. Consider, for example,

Table 1: **Asymptotic Order of Residual**

Type of Zone	Order of Residual $u_t + f(u)_x$	Local Coordinates ξ	τ
Regular zone	$O(\epsilon)$	x	t
Shock layer	$O(\epsilon^{-1})$	$(x - S(t))/\epsilon$	t
Weak singularity	$O(\epsilon^{1/2})$	$(x - S(t))/\epsilon^{1/2}$	t
Shock interaction with other singularities	$O(\epsilon^{-1})$	$(x - S_0 - S_1 t)/\epsilon$	$(t - t_o)/\epsilon$
Discontinuity with f locally linear	$O(1)$	$(x - S_0 - S_1 t)/\epsilon^{1/2}$	$(t - t_o)$
Formation of shock	$O(\epsilon^{-1/4})$	$(x - S_0 - S_1 t)/\epsilon^{3/4}$	$(t - t_o)/\epsilon^{3/4}$

the equation

$$\frac{\partial U}{\partial t} + \frac{\partial}{\partial x} F(U) = \epsilon \frac{\partial}{\partial x} \left(P(U) \frac{\partial U}{\partial x} \right). \tag{1}$$

The solution of the inviscid problem

$$\frac{\partial U}{\partial t} + \frac{\partial}{\partial x} F(U) = 0, \tag{2}$$

can exhibit some singularities such as shocks, weak discontinuities that propagate along the characteristics, and interaction of singularities. For each singularity corresponds a thin layer, where the viscous perturbation cannot be neglected. One can identify, using a matched asymptotic technique, the order of magnitude of the residual and the scaling of the layer for each type of singularities in the scalar case (cf. Table 1).

In particular, this result holds for a shock layer in the case of a system of conservation laws. When we use a hyperbolic scheme, for example a Godunov scheme, to compute a conservation law with or without viscosity, one can use this information to identify the zone of a shock, based on the computation of the residual. This may require the use of two grids; however, we can identify three categories of points depending on whether it is a regular zone, a shock, or something else. Layers that correspond to weak singularities can be solved using a regular correction technique as in [11] with eventually some adaptivity. Interaction of singularities need a stretching in time and space in the subdomain according to Table 1. We will emphasize here the numerical treatment of the *shock layer.* based on the asymptotic technique of matching [7]. We refer to [4] and [9] for more details about the method and some numerical experiments.

Now we are going to describe the method extended to the following simplified model of reacting flow of Majda

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}[f(u) - q_o Z] = \epsilon \frac{\partial^2 u}{\partial x^2}, \tag{3}$$

$$Z_x = \varepsilon^{-1} \phi(u) Z, \tag{4}$$

where $\phi(u) = 1$ if $u > 0$, and $\phi(u) = 0$ elsewhere. We refer to [13] for the derivation of this model and its precise statement.

This model belongs to the following class of diffusion-convection-reaction problems

$$-\varepsilon\frac{\partial}{\partial x}(P(u)\frac{\partial u}{\partial x})+\frac{\partial u}{\partial t}+\frac{\partial}{\partial x}F(u)+D(u,\varepsilon)=0, \tag{5}$$

when $D(u,\varepsilon)$ is of order 1 except possibly in some transition layer. if $D(u,\varepsilon)$ is uniformly bounded, $D(u,\varepsilon)$ occurs as a regular perturbation in a shock layer (i.e., the source terms appear only as a correction in the second order term of the inner expansion). Therefore, the asymptotic analysis of a shock layer extended to (5) has only some minor modifications.

We will emphasizes the case when $D(u,\varepsilon)$ balances the viscosity in a transition layer, that is $D(u,\varepsilon)\sim\varepsilon^{-1}D_1(\hat{u})$ with $D_1(\hat{u})=O_s(1)$. We will refer to this case as a *reacting shock layer.*

The first order term in this layer satisfies the ODE problem

$$\begin{cases} -\frac{\partial}{\partial\xi}\left(P(\hat{U}^0)\frac{\partial\hat{U}^0}{\partial\xi}\right)+\frac{\partial}{\partial\xi}\left(F(\hat{U}^0)-S'(t)\hat{U}^0\right)+D_1(\hat{U}_0)=0, \\ \hat{U}^0\to U_l^0 \quad \text{as } \xi\to-\infty, \\ \hat{U}^0\to U_r^0 \quad \text{as } \xi\to+\infty, \end{cases} \tag{6}$$

Thus, the R & H relation becomes the following jump condition;

$$\left[\!\left[F(\hat{U}_0)-S'(t)\hat{U}_0\right]\!\right]+\int_{U_l}^{U_r}D_1(\hat{U})d\hat{U}=0$$

In particular, a hyperbolic scheme applied to (5) will not in general give the right speed of propagation for a reacting shock layer, since the numerical viscosity of the scheme will interact with the source term.

The asymptotic analysis of a reacting shock layer for the *Majda problem* shows that the first order term in the layer satisfies

$$\begin{cases} \hat{U}_{0,\xi}=H(\hat{U}_0,\hat{Z}_0)-H(U_{l/r},Z_{l/r}), \\ \hat{Z}_{0,\xi}=\phi(\hat{U}_0)\hat{Z}_0, \\ \\ \phi(U_l)=1;\phi(U_r)=0, \\ \hat{U}_0\to U_{l/r} \quad \text{as } \xi\to\mp\infty, \\ \hat{Z}_0\to 0 \quad \text{as } \xi\to-\infty, \\ \hat{Z}_0\to 1 \quad \text{as } \xi\to+\infty, \end{cases} \tag{7}$$

where $H(u,z)=1/2u^2-S'(t)u-q_0Z$.

The ability to construct the layer supposes the jump condition:

$$1/2U_l^2-S'(t)U_l=1/2U_r^2-S'(t)U_r-q_0,$$

and that there exists a trajectory of (7) from $(U_l,0)$ to $(U_r,1)$. An extensive study of (7) is given in [13].

One obtains the shift in $\hat{U}_0$ using the conservation relation

$$\frac{\partial}{\partial t}\int_{\mathbb{R}} u_{as} = q_0 - [F(U)]_{U_l}^{U_r} + 0(\epsilon) \tag{8}$$

Now, we present the numerical method based on these results. We start from the following elementary finite difference scheme

$$\begin{cases} \frac{U_{i+1}^{n+1}-U_i^n}{\Delta t} = \epsilon\frac{U_{i-1}^n-2U_i^n+U_{i+1}^n}{\Delta x^2} - \frac{F(U_{i+1}^n)-F(U_{i-1}^n)}{2\Delta x} + q_0\,\frac{Z_{i+1}^n-Z_{i-1}^n}{2\Delta x}, \\ \\ \frac{Z_i^{n+1}-Z_{i+1}^{n+1}}{\Delta x} = K\,\phi(U_{i+1}^{n+1})\,Z_{i+1}^{n+1}. \end{cases}$$

This explicit scheme can be improved by using a Riemann solver to compute the flux. However, for our purpose, we do not need a more sophisticated scheme as long as it is a conservative scheme. We are interested in a reacting shock layer; so, our numerical test identifies the zone of strong singularities where *both* the viscosity and the reaction terms are of order ϵ^{-1}.

As in [4], we obtain U_l, U_r, and some approximation of the position of the interface. Let us notice that in our numerical experiment, we solve a Riemann problem and U_l, U_r are independent of time. Therefore, $\hat{U}_0$ is the only nonzero term of the reacting shock layer.

A solution (U_0, Z_0) of (5) is then computed with any ODE scheme. One can use some asymptotics in the neighborhood of critical points $(U_{l/r}, Z_{l/r})$ to derive explicit formulae to decrease the cost of the computation of $(\hat{U}_0, \hat{Z}_0)$.

Then, one substitutes to (U_i^n, Z_i^n) in the reacting shock layer, the only traveling wave $(\hat{U}_0, \hat{Z}_0)$ that satisfies the conservation relation (8).

We have implemented this domain decomposition method for the spiked strong detonation case with $U_l = 1.0$, $U_r = -1.5$, and $q_0 = 2.375$. We use 40 points in the regular grid to solve the problem with $\epsilon = 0.05$ (Fig. 1). Numerically, the thickness of the layer is about 12ϵ. One can see the ϵ jump at the interface between the inner domain and the outer domains. We obtain some analogous results with 400 points in the regular grid and $\epsilon = 0.005$ (Fig. 2). Because U_l and U_r are so easy to obtain numerically, there is no significant error in the speed of propagation of the layer. We intend to solve more difficult cases in the future that requires the solution of the next order term in the inner expansion.

The problem of the initial formation of this reacting shock layer will be solved with the domain decomposition method presented in the next section.

We can also apply the minimum viscosity method of [4] to this problem in a straightforward way. We keep only one artificial point in the layer to allow the scheme to be conservative. The figures 3 and 4 shows the result with 40 and 400 points, respectively. In each case, the composite scheme tracks the interface with an error less than the mesh size.

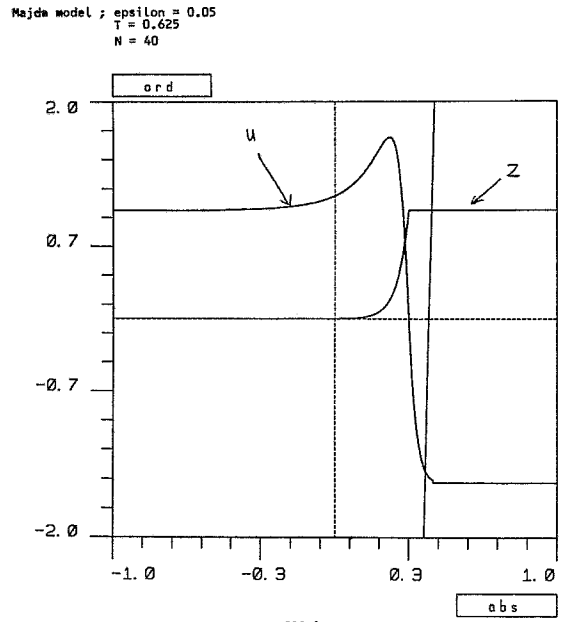
Majda model ; epsilon = 0.05
T = 0.625
N = 40
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FIG 1

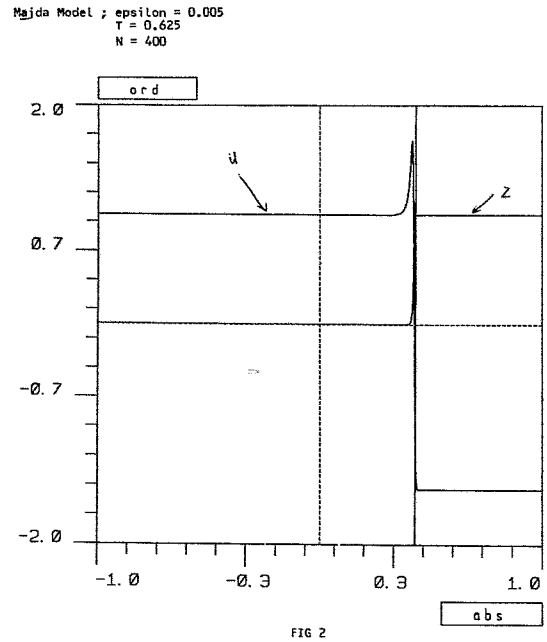
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FIG 2

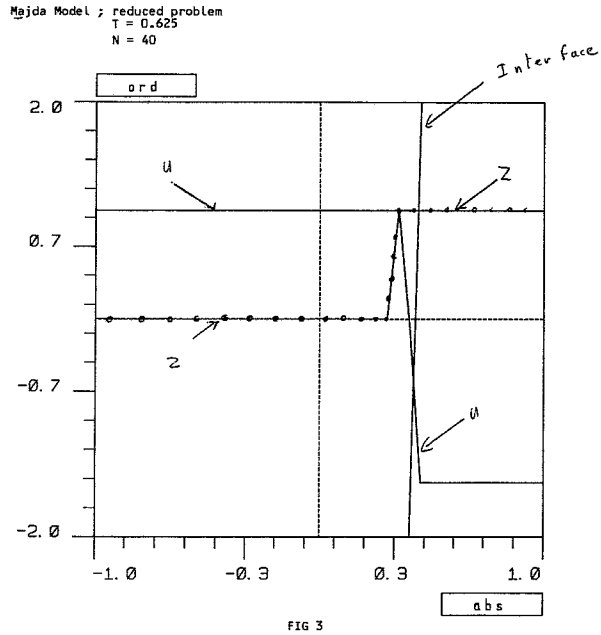
Majda Model ; reduced problem
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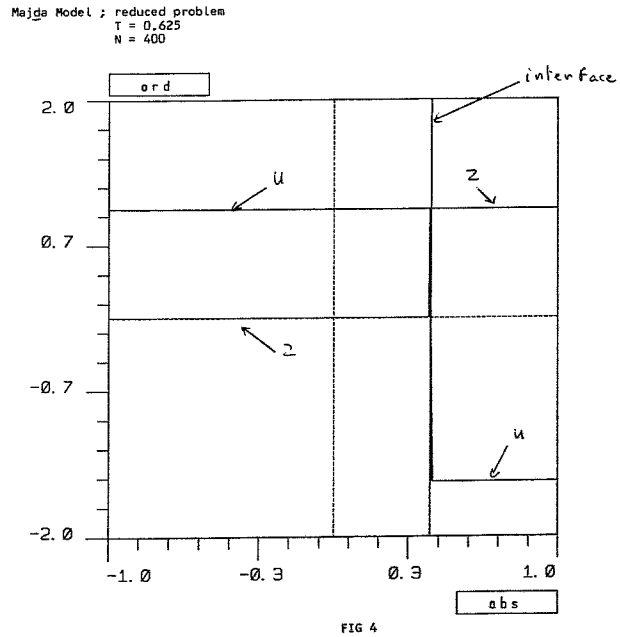
FIG 3


Majda Model ; reduced problem
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N = 400
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FIG 4

3 Adaptive domain decomposition with pseudospectral

When solving a regular problem with domain decomposition and a fixed total amount of collocation points, the accuracy decreases as the number of domains increases. This is characteristic of the pseudospectral accuracy. However, for stiff problems, numerical experiments demonstrate that one can drastically improve the numerical accuracy of the pseudospectral approximation by adapting domain decomposition. This adaptivity is based on the a priori estimates of [3].

By using the information given in the asymptotic analysis to localize the layers and obtain the magnitude of the mapping parameters for each type of layer, one reduces the cost of adaptivity. In singular perturbation theory [7], one introduces subdomains and stretching variables to solve these layers, and one obtains a uniform approximation of the solution. We will use some analogous tools in the numerical method that follows.

We introduce two one-parameter families of mappings [3],

$$\begin{array}{ccc} [-1,1] & \longrightarrow & [-1,1], \\ s & & y = f_i(s,\alpha), \end{array} \tag{9}$$

with $f_1(s,\alpha) = \pm\left[\frac{4}{\pi}\text{atan}(\alpha\ \tan(\frac{\pi}{4}(\pm S-1))+1\right]$, and $f_2(s,\alpha) = \alpha\text{tan}(s\ \text{atan}(\alpha^{-1})$. α is a small free parameter that describes how one concentrates the collation points in the physical space.

We call f_1 a mapping of BL type and f_2 a mapping of TL type. We use in f_1 a + sign (respectively, a − sign) for a BL on the right (respectively, on the left) of the interval. A number of other mappings are possible choices but we restrict ourselves to the previous examples.

In singular perturbation, one uses stretching variables of the form $\xi = \frac{x-x_k}{\epsilon}$, where x_k is the location of the layer, and ϵ is a measure of the stretching. It is easy to see that the parameter α in the nonlinear mappings f_1 and f_2 plays a role analogous to ϵ in the numerical method. One needs also to focus the stretching on a subdomain $[x_k-L_k, x_k+L_k]$ of Ω. So we introduce a second one-parameter family of affine mappings. To solve a TL we use

$$\begin{array}{ccc} [-1,1] & \longrightarrow & [x_k - L_k, x_k + L_k], \\ y & & x = g_k(y, L_k), \end{array} \tag{10}$$

and to solve a BL on the right, for example, we use

$$\begin{array}{ccc} [-1,1] & \longrightarrow & [x_k - L_k, x_k] \\ y & & x = g_k(y, L_k). \end{array} \tag{11}$$

Difficult problems include the computation of the free parameter α characteristic of the stretching, and also the localization of the layer (i.e to compute x_k or L_k). We have two

tools at our disposal. The first tool is the asymptotic analysis of the PDE involving a critical parameter. This tool is strongly related to the PDE, so we emphasize this aspect when we study specific examples. The second tool is relevant for the approximation theory, and requires a purely automatic treatment (see [2] [3]). We present in [10] these tools in the context of an arbitrary number of subdomains to solve singular perturbation problems.

It is quite clear that the Chebyshev Method solves a BL more easily than a TL because of the $O(N^2)$ concentration of the collocation points at both ends of the interval $[-1,1]$. When the Chebyshev Method is supplemented with a mapping of BL-type, one improves the (already good) numerical accuracy of the approximation when the problem has boundary layers. However, it is unclear what the best mapping and subdomain technique is for a TL.

As a matter of fact, let us suppose that u exhibits a single TL at $x_0 \in \Omega$. One can use either

- two subdomains with their mapping of BL type and their interface in x_0, or
- three subdomains with an inner domain centered at x_0 and its mapping of TL type.

We have tested these two strategies to adapt and split the domain on the Majda simplified model of reacting flow.

We have applied the domain decomposition technique [12] with pseudospectral on the initial boundary value problem (5) on the domain $[a,b]$ with the initial condition

$$u(x,0) = (U_l - U_r)\frac{1-\tanh(\xi)}{2} + U_r, \quad rm for\ \xi = \frac{x}{\varepsilon},$$

and the boundary conditions

$$U(a) = U_l,\ U(b) = U_r.$$

We report here some numerical experiments of the spiked strong detonation case of Section 2 with $U_l = 1$, $U_r = -1.5$, $q_0 = 2.375$ and $a = -6$, $b = 8$. Our numerical scheme explicitly solves the nonlinear convection term $(\frac{u^2}{2})_x$, therefore the time step is limited by the CFL condition. Also we impose the piecewise Chebyshev approximation of $u(x,.)$ to be C^1 at the interface. We found it to be more accurate, robust and easy to adopt the two subdomain strategy to solve for the reactive shock layer. Numerical evidence of this result (as well as asymptotic analysis) are reported in the companion paper [10]. Also it is very convenient and efficient to move the interface by tracking the maximun of the Arrhenius term $q_o\varepsilon^{-1}\Phi(u)Z$. The numerical method solves the initial formation of the reactive shock layer and then the solution converges to the traveling wave (6) as t grows.

We have obtained a numerical error of ordre one per cent on the maximum value of u and on the speed of propagation of the traveling wave for $\varepsilon = 0.1$ (respectively, $\varepsilon = 0.01$) with 20 (respectively, 42) collocation points per subdomain (see Fig. 5 and 6). One observes that the method is conceptually very well adapted to solve the initial formation of the layers as well as the interaction of singularities. However, because of the CFL constraint,

and because the minimum distance between two discretization points has to be of order less than ϵ in the layer, this method is computationally expensive to solve for a traveling wave.

A further step in our research is to implement a domain decomposition method that is a mixture of both methods presented in this paper. Strong singularities, such as a simple shock or a reactive shock that are easily identified, can be solved by the first domain decomposition technique presented in this paper. Interaction of singularities or initial layers may be solved by the adaptive domain decomposition based on pseudospectral techniques. In addition, at each stage of the computation, one may use asymptotics to select the best method.

Let us mention that to extend the method to solve problems in two space dimensions, one has to use domain decomposition to solve layers as well as the difficult problem of geometry due to the curvature of the fronts. Also we may expect both domain decomposition methods to be useful tools for parallel computing of singularly perturbed problems in two space dimensions.

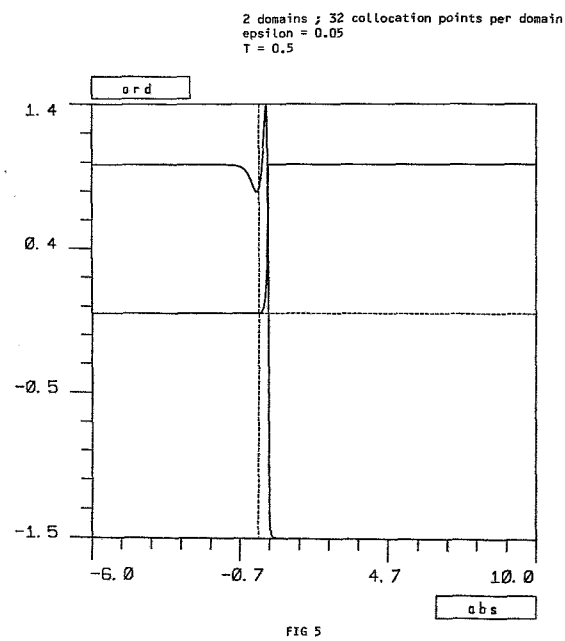

FIG 5

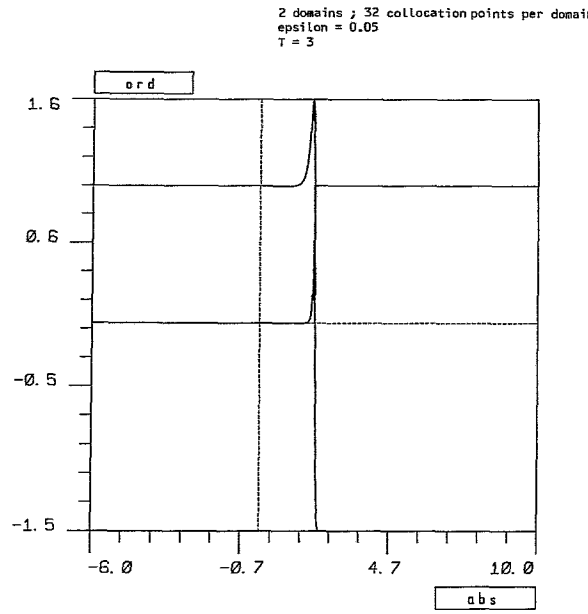

FIG 6

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