A CHARACTERISTICS BOX SCHEME FOR THE SINGULARLY PERTURBED CONTINUITY EQUATION

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Abstract.

A new scheme is introduced for discretising the continuity equation. The scheme approximately satisfies the requirement that the reduced difference equation is a backward Euler integration for the characteristics problem of the reduced continuity equation.

1. INTRODUCTION

The connection between singular perturbation theory and the semiconductor equations has already been indicated in [1]. However only the case of the Poisson equation was considered. Although this in our opinion is correct, the character of the continuity equation is even more important in this respect. The amazing fact is that the 1-D discretisation derived by Scharfetter-Gummel is essentially the same as the scheme derived by Il'yin [2]. The reasoning in both cases is completely different but only valid for one-dimensional problems. This reasoning is not as such valid in two dimensions. Basically this is owing to the fact that the 1-D reasoning depends on the existence of two functions spanning the solution space of a one dimensional case. In two dimensions we need an infinity of basic solutions.
However in this paper we present a new discretisation using the one dimensional reasoning in a correct way.
The basic idea is the following: The dominant part in the continuity equation is first order. A first order equation may be considered as a set of ordinary differential equations along the characteristics. These should be integrated in a stable way. The characteristics point of view makes it possible to use the one dimensional reasoning again.

In section two we briefly discuss singularly perturbed problems, in section three we consider the continuity equation from this point of view, in section four the 2-D scheme is derived and in section five this is applied to the continuity equation. In [3], an accompanying paper, some further aspects are treated.

2. SINGULARLY PERTURBED 3-D PROBLEMS

In this section we briefly discuss singularly perturbed problems. A thorough treatment can be found in [4] and [5].

Consider the equation

$$y''+ay'=r \tag{2.1}$$

on [0,1]. For very large 'a' this equation closely resembles

$$ay'=r \tag{2.2}$$

However for (2.1) we have two boundary conditions whereas (2.2) is an initial value problem. So for large 'a' it seems that we have one boundary condition too many. This is found back in a transition layer in the solution. It is as if the second boundary condition is discovered in a short interval. This can also be understood by considering the solution in the form

$$\alpha+\beta e^{-ax}+f(x)$$

where f(x) is a solution of the inhomogeneous problem not satisfying the boundary conditions. The $e^{-ax}\not\approx 0$ only in a very short interval.

The difference scheme used for (2.1) must be adapted to the fact that we are almost solving ay'=r for large 'a'. If for instance we use

$$(\delta_h^2+ah\delta_{2h})y=h^2r$$

for (2.1) (for notation see e.g. [6]). We find

$$\delta_{2h}y=h^2r$$

for (2.2). It is obvious that this is not a stable ODE integrator, which we would wish. This leads to the following

requirement (A): the difference scheme for (2.1) must reduce to a stable scheme for (2.2) of $a \longrightarrow \infty$. In [2] a scheme is derived which has this property. To understand this scheme we may reason as follows. The operator δ_{2h} should be replaced by an operator resulting in backward Euler for (2.2). However depending on the sign of 'a' this should by Δ or ∇. We would also like to have δ_{2h} for small 'a'.
A convex combination

$$D(a)=.5((1+s(a))\Delta+(1-s(a))\nabla)$$

can be used for this purpose. We still have to find a suitable function s(a). It has also been observed that the transition layer may be understood via the behaviour of the solution e^{-ax} of the homogeneous problem. So by substituting e^{-ax} in the difference scheme

$$(\delta^2+ahD(a))y=0 \tag{2.3}$$

we find the function s(a).

Realising that $\Delta+\nabla=\delta_{2h}$ and $\Delta-\nabla = \delta_n^2$ we may rewrite this as

$$\delta_h(\gamma\delta_h+.5ah\mu)y=0 \tag{2.4}$$

with $\gamma=(1+ahs(a))=.5ah\ \mathrm{cotgh}(.5ah)$. And indeed this satisfies the requirements.
The important observation is that we have used the fact that the homogeneous scheme has two basic solutions, 1 and e^{-ax} in an essential way. This can not be extended to two dimensions.

3. THE 1-D CONTINUITY EQUATION

The continuity equation for p may be written as

$$\mathrm{div\ grad}\ p+\mathrm{grad}\psi\ .\mathrm{grad}\ p=R-p\ \mathrm{div\ grad}\psi=\bar{R} \tag{3.1}$$

In one dimension this gives

$$p_{xx}+\psi_x p=R \tag{3.2}$$

an equation of the same type as (2.1). For ψ_x large, as may be the case in a depletion layer, this equation is singularly perturbed.
It can easily be checked that any other choice of variables gives exactly the same first order term in the equation. So (2.4) leads to

$$\delta_n(\gamma\delta_n+.5\psi_x h\mu)p=R(p,\psi) \tag{3.3}$$

It should be noted that the straight forward translation of (2.4) in (2.5) used the fact that 'a' is constant. For non constant 'a' a slightly different derivation is needed.

4. 2-D SINGULARLY PERTURBED PROBLEMS

Consider

$$\text{div grad } y+E.\text{grad } y=r \tag{4.1}$$

in 2D, If E is very large this equation will resemble

$$E.\text{grad } y=r \tag{4.2}$$

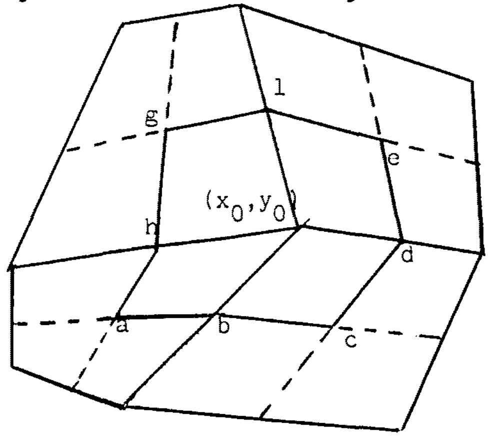
This equation may be considered as defined by a set of ODE's along the characteristics (see e.g. [7]). This allows us to reintroduce a one dimensional reasoning. Then we replace requirement (A) by

requirement (B): the discrete scheme for (4.1) must reduce to a stable scheme for the ordinary differential equations along the characteristics defined by (4.2) if $\|E\| \to \infty$

6. THE 2-D CONTINUITY EQUATION

In this section we give a scheme for the 2-D continuity equation which satisfies requirement (B) for each mesh if the characteristics are straight lines. Of course in realistic problems characteristics are not straight lines. However in that case we cause an approximation error which may be lowered by changing interpolations. It should be noted that neither the upwind FEM schemes nor the usual 2D Scharfetter-Gummel satisfy this requirement.

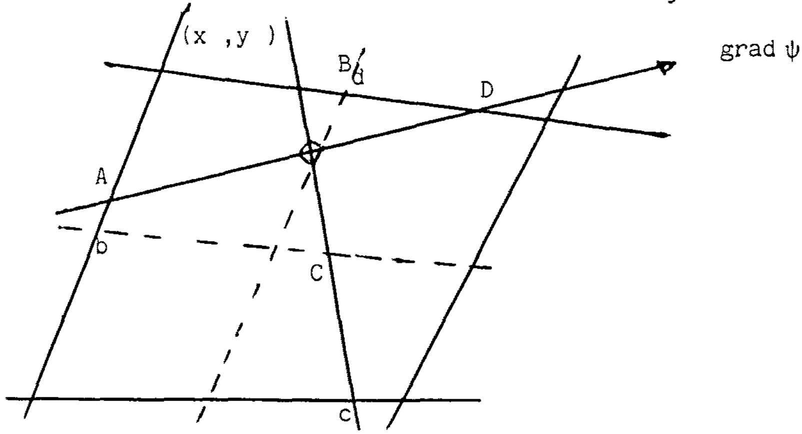
Suppose we have a quadrilateral mesh. Let us consider four neighbouring meshes as shown in fig 1.



We construct a box around the midpoint (x_0, y_0) by using the connections of the midpoints of mesh segments. This gives the octogon G=abcdefgh with boundary Γ. Then we use a Green's theorem as usual in box schemes giving

$$\int_\Gamma \text{grad } p + p.\text{grad } \psi . dn = \int_G \tilde{R}$$

For any quadrature we now must establish (grad p+p gradψ).n in the quadrature points. We use a local coordinate system (x', y') in the quadrature points with one axis along grad ψ , i.e. tangential to the characteristics. For one box this is shown in fig 2.



This gives four points A, B, C and D as cross-section for the local coordinate system and the meshlines. In these local coordinates the equation has the form

$$\int_\Gamma (p_{x'} + \psi_{x'} p + p_{y'}) . n = \int_G \tilde{R}$$

So it is sufficient to apply the one dimensional reasoning only for $p_{x'} + \psi_{x'} p$ only in this case. However, then we need values in the points A, B, C and D. For this we express those values in terms of the nodal unknown via linear interpolation. The effect of this choice on the order of the approximation still has to be investigated. However it is obvious that a variety of choices for the quadrature and interpolation is now possible.

If ψ_x is very large this scheme is, except for the errors introduced by the linear interpolation of the A, B, C and D values and the error introduced by the curvature of the characteristics, backward Euler for the ordinary differential equations involved.

CONCLUDING REMARKS

We have implemented this scheme in our program package CURRY and have used it to investigate several realistic devices. A simple one dimensional example suffices to show the practical importance of the scheme. Consider the two meshes given in fig 3.

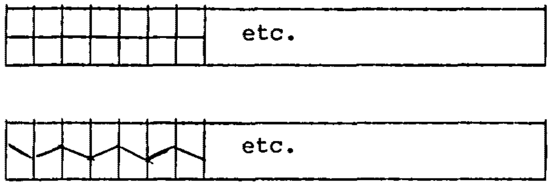


fig. 3

They were used to discretise a one dimensional diode problem [8]. Using the classical Scharfetter-Gummel approach gave an essential discrepancy between the solutions. This discrepancy increased when the difference between the meshes was increased. Using the new scheme gave exactly the same result, independant of the mesh used.

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