SUFFICIENT CONDITIONS FOR UNIFORM CONVERGENCE OF A DIFFERENCE SCHEME FOR A SINGULARLY PERTURBED PROBLEM IN CONSERVATION FORM

Paul A. Farrell

Computing Dept., College of Commerce, Rathmines, Dublin 6.
Numerical Analysis Group, Trinity College, Dublin 2.

We shall consider a number of families of difference schemes for the solution of a two-point boundary value problem in conservation form and deduce conditions on their coefficients sufficient for uniform convergence. We shall also show that the well known Scharfetter-Gummel scheme for the continuity equations in semi-conductor devices is a member of one of these families.

We shall consider the following problem

$$\varepsilon(p(x)u_\varepsilon'(x))' + (q(x)u_\varepsilon(x))' - r(x)u_\varepsilon(x) = s(x) \quad 0 < x < 1 \tag{1}$$

$$u_\varepsilon(0) = A \quad , \quad u_\varepsilon(1) = B$$

with the following conditions on the coefficients

$$\bar{p} > p(x) \geq \underline{p} > 0 \quad , \quad p'(x) \geq 0 \tag{2}$$

$$q(x) \geq \underline{q} > 0 \quad , \quad q' \leq 0 \quad , \quad r(x) \geq 0 \; .$$

These conditions are sufficient to guarantee that there exists a maximum principle for the problem from which we may deduce stability of the solution.

We remark that the derivation of meaningful sufficient conditions for problems in conservation form is more difficult than in the non-conservative form. This arises in part because schemes for such problems should be of essentially "centered" difference form to preserve the conservation properties of the original equation. The derivation of sufficient conditions on the other hand depends on casting the difference equation in "upwinded" form so that the solution of the reduced difference equation is stable and a good approximation to the solution of the reduced differential equation. Thus, for convenience in deducing the sufficient conditions, we transform (1) to the non-conservative form :

$$\varepsilon u_\varepsilon''(x) + a(x)u_\varepsilon'(x) - b(x)u_\varepsilon(x) = f(x) \; , \; 0 < x < 1 \tag{3}$$

BAIL III. Proceedings of the Third International Conference on Boundary and Interior Layers - Computational and Asymptotic Methods, (J.J.H. Miller ed.), Boole Press, Dublin, (1984).

where

$$a(x) = \frac{q(x) + \varepsilon p'(x)}{p(x)} \quad , \quad b(x) = \frac{r(x) - q'(x)}{p(x)} \quad , \quad f(x) = \frac{s(x)}{p(x)} \tag{4}$$

Note that in this form $a(x)$ is a function of ε as well as x. In this case, rewriting in terms of $t = x/\varepsilon$ we see the first boundary layer equation is just

$$v_{tt}(t) + \frac{q(0)}{p(0)} v_t(t) = 0$$

Thus the $\varepsilon p'(x)/p(x)$ term plays no part in determining the first boundary layer function. We may thus prove the following generalisation of Lemma 2.4 of [4].

<u>Lemma 1</u>

Let $u_\varepsilon(x)$ be the solution of (1),(2) then

$$u_\varepsilon(x) = \gamma v(x) + z(x)$$

where $v(x) = e^{-q(0)x/p(0)\varepsilon}$, $|\gamma| \leq C_1$ and

$$| z^{(i)}(x) | \leq C(1 + \varepsilon^{-i+1} e^{-\underline{q}x/4\bar{p}\varepsilon}) \qquad 1 \leq i \leq k+1.$$

Let us now consider a difference scheme for the modified problem (3):

$$\varepsilon_i^+ D_+ D_- u_i^h + a_i^h D_+ u_i^h - b_i^h u_i^h = f_i^h \tag{5}$$

$$u_0^h = A \qquad u_N^h = B$$

Sufficient conditions for this difference scheme to be uniformly convergent are given by the following lemma.

<u>Lemma 2</u>

If a difference scheme has the form (5) where $\varepsilon_i^+ = \varepsilon\sigma_i^+$, a_i^h , b_i^h , f_i^h are bounded and satisfy the conditions

$$\varepsilon_i^+ \geq 0 \quad , \quad a_i^h \geq \underline{a}^h > 0 \quad , \quad b_i^h \geq 0 \tag{I}$$

$$| a_i^h - a(x_i) | \leq Ch \tag{II}$$

$$| b_i^h - b(x_i) | \leq Ch \tag{III}$$

$$| f_i^h - f(x_i) | \leq Ch \tag{IV}$$

and for any given $\bar{x}$ s.t. $0 < \bar{x} \leq 1$

$$|\sigma_i^+ - \sigma(a(0)\rho)| \leq C\rho w(\rho) x_i e^{-q(\zeta)\rho/p(\zeta)} + Ch\sigma(a(0)\rho) \quad 0 \leq x_i \leq \bar{x} \tag{Va}$$

where $0 \leq \zeta \leq x_i + Ch$, $w(\rho)$ is a polynomial in ρ and $\sigma(z) = \dfrac{z}{e^z - 1}$

$$\text{and} \qquad |\varepsilon_i^+ - \varepsilon| \leq Ch \qquad \bar{x} \leq x_i \leq 1 . \tag{Vb}$$

then (5) is uniformly convergent of order h to the solution of (3),(4),(2) for all $h \leq h_0 < \bar{x}$.

Proof: This is a slight generalisation of the proofs in [2],[3]. We consider v(x) and z(x) seperately and bound the truncation error due to each by

$$C\,(h + \min(1,\rho) e^{-\underline{q} x_i / 4\bar{p}\varepsilon}).$$

We then use the maximum principle to obtain a bound on the error.

We would now like to formulate families of difference schemes for the original problem (1), rather than (3), and deduce conditions on the coefficients of these schemes sufficient for uniform convergence.

Consider first the following family of schemes

$$\varepsilon\delta(\sigma_i p_i^h \delta u_i^h) + \delta(q_i^h \mu u_i^h) - r_i^h u_i^h = s_i^h \tag{6}$$

$$u_0^h = A \qquad , \qquad u_N^h = B$$

where

$$\delta z_i = (z_{i+1/2} - z_{i-1/2})/h \quad .$$

$$\mu z_i = (z_{i+1/2} + z_{i-1/2})/2 \quad .$$

For this family of schemes we have the following sufficient conditions.

Theorem 1

The following conditions on the coefficients of (6) are sufficient for uniform convergence of at least order 1.

(cI) The scheme (6) is uniformly stable,

(cII) $|p_{i-1/2}^h - p(x_{i-1/2})| \leq Ch$

(cIII) $|q_{i-1/2}^h - q(x_{i-1/2})| \leq Ch$, $|\delta[q_i^h - q(x_i)]| \leq Ch$

(cIV) $|r_i^h - r(x_i)| \leq Ch$

(cV) $\qquad |s_i^h - s(x_i)| \le Ch$

(cVIa) $$\left|\sigma_{i-1/2} - \frac{\rho q_{i-1/2}^h}{2p_{i-1/2}^h} - \sigma(q(0)\rho/p(0))\right|$$

$$\le C\rho\omega(\rho)x_i\, e^{-p(\zeta)/q(\zeta)\rho} + Ch\sigma(q(0)\rho/p(0)) \quad , \quad 0 \le x_i \le \bar{x}$$

where $0 \le \zeta \le x_i + Ch$, $\omega(\rho)$ is a polynomial in ρ and $\sigma(z) = \dfrac{z}{e^z - 1}$ as before and

(cVIb) $\qquad |\varepsilon\sigma_i - \varepsilon| \le Ch \qquad , \qquad \bar{x} \le x_i \le 1$.

Proof: Rewriting this scheme in the form (5) we obtain

$$\sigma_i^+ = \left(\sigma_{i-1/2} - \frac{\rho q_{i-1/2}^h}{2p_{i-1/2}^h}\right)p_{i-1/2}^h/p(x_i)$$

$$a_i^h = (\varepsilon\delta(\sigma_i p_i^h + \mu q_i^h)/p(x_i)$$

$$b_i^h = (r_i^h - \delta q_i^h)/p(x_i) \quad , \quad f_i^h = s_i^h/p(x_i)$$

It is easily verified that the conditions of Lemma 2 are satisfied and hence the scheme is uniformly convergent.

An alternative family of difference schemes for (1) is given by the following formulation.

$$\varepsilon\sigma_i\delta(p_i^h\delta u_i^h) + D_0(q_i^h u_i^h) - r_i^h u_i^h = s_i^h \quad , \quad 1 < i < N \tag{7}$$

The conditions for this formulation are the same except for (cIII) and (cVIa) which are replaced by :

(cIII) $\qquad |q_i^h - q(x_i)| \le Ch \quad , \quad |D_0[q_i^h - q(x_i)]| \le Ch$

(cVIa) $$\left|\sigma_i - \frac{\rho q_{i-1}^h}{2p_{i-1/2}^h} - \sigma(q(0)\rho/p(0))\right|$$

$$\le C\rho\omega(\rho)x_i\, e^{-p(\zeta)/q(\zeta)\rho} + Ch\sigma(q(0)\rho/p(0)) \quad , \quad 0 \le x_i \le \bar{x}$$

Similarly we could propose a number of other formulations and deduce sufficient conditions for uniform convergence. The family of schemes given by (6) is more natural than that given by (7) since (cVIa) and the requirement for stability imply that σ_i should be a function of $\rho q_i^h/2p_i^h$ which is a more natural form than in the case of (7).

A particular example of each family was given in Part II, Sect. 9 of [1] and a proof of uniform convergence was given for the member of family (7). The scheme of type (6) is given by:

$$\varepsilon\delta(\sigma_i p(x_i)\delta u_i^h) + \delta(q(x_i)\mu u_i^h) - r(x_i)u_i^h = s(x_i) \tag{8}$$

where

$$\sigma_i = Y_i \coth Y_i \qquad \text{and} \qquad Y_i = \frac{\rho q(x_i)}{2p(x_i)}.$$

O'Riordan and Stynes [5] deduced a scheme, for the case $b(x) \equiv 0$, using the finite element method and showed that it is uniformly convergent of order h^2. It can be easily verified that this scheme also satisfies the conditions of Theorem 1. Numerical results also verify that (8) is uniformly convergent of order h whereas this scheme is uniformly order h^2. Graphs of the results for both schemes are given in Fig. 1 and Fig. 2.

Fig 1

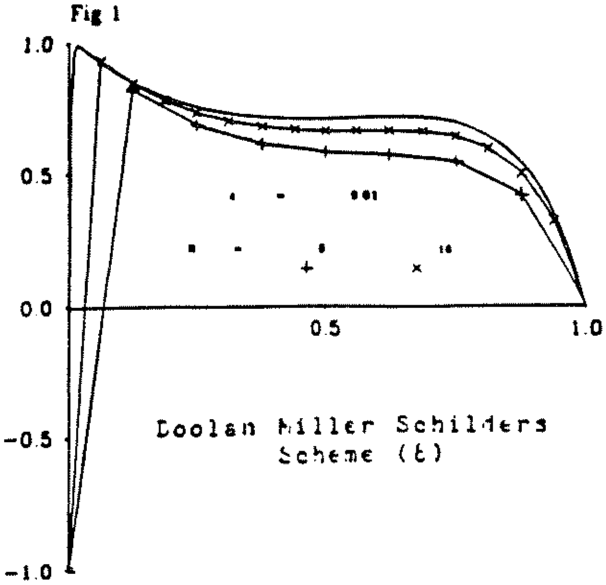
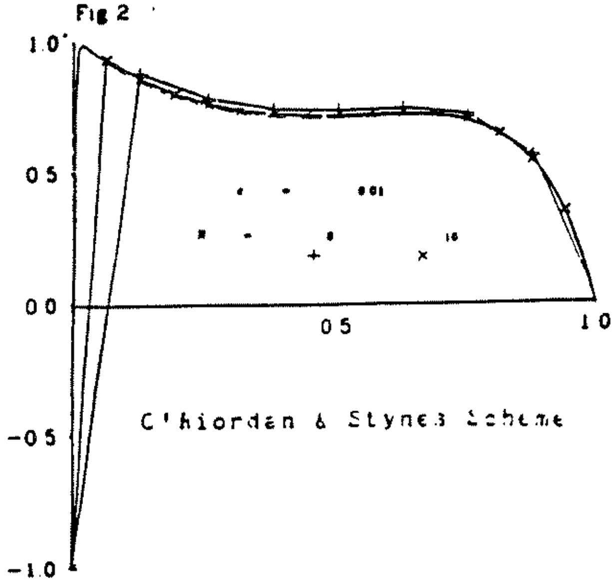


Fig 2



$\varepsilon((1+x^2)u'(x))' + ((4-2x-x^2)u(x))' = -4(3x^2-3x+1)((x-.5)^2+2)$

$u(0) = -1,\ u(1) = 0$

A Practical Application

It is well known that classical methods are unsatisfactory for the solution of the continuity equations in semi-conductor devices. Using the formulation in terms of electron densities the equation after scaling and assuming zero recombination is:

$$(n' - \psi' n)' = 0 \quad . \tag{9}$$

Using this scaling Markowitz et al.[6] have shown that the Poisson equation is a singularly perturbed equation with small parameter λ of order 10^{-5}. In this scaling (assuming the interface is at $x = 0$)

$$| \psi'(x) | \leq C \lambda^{-1} e^{-C|x/\lambda|} \quad .$$

Thus $\psi'(x)$ in (9) is unbounded as λ approaches 0 and multiplying by λ we get:

$$(\lambda n' - q n)' = 0 \quad . \tag{10}$$

where $q(x) = \lambda\psi'(x)$ is a bounded function. Thus the continuity equation is also a singularly perturbed problem in conservation form.

The mathod used widely in the literature to solve this equation is known as the Scharfetter-Gummel mathod and is given by:

$$D_+ J_{i-1/2} = 0 \quad \text{where} \quad J_{i+1/2} = - D_+\psi_i \left(\frac{n_{i+1}}{1 - e^{hD_+\psi_i}} + \frac{n_i}{1 - e^{-hD_+\psi_i}} \right) \quad .$$

Now it is easily shown that this is equivalent to the scheme (8), with $p(x) \equiv 1$ and $r(x) = s(x) \equiv 0$, provided we take the natural approximation for $q(x) = \lambda\psi'(x)$ that is:

$$q^h_{i+1/2} = q(x_{i+1/2}) = \lambda\delta\psi_{i+1/2} \ .$$

<u>References</u>

[1] E.P. Doolan, J.J.H. Miller, W.H.A. Schilders, "Uniform numerical methods for problems with initial and boundary layers", Boole Press, Dublin (1980)

[2] P.A. Farrell, "Uniformly Convergent Difference Schemes for Singularly Perturbed Turning and Non-Turning Point Problems", Ph.D. Thesis, Trinity College Dublin.

[3] P.A. Farrell, "Necessary and Sufficient Conditions for Uniform Convergence of a Difference Scheme for a Non-Turning Point Problem", (to be published).

[4] R.B. Kellogg, A. Tsan, "Analysis of some difference approximations for a singular perturbation problem without turning points", Math. Comp., 32, pp. 1025-1039 (1978)

[5] E. O'Riordan, M. Stynes, "A Finite Element Method for a Singularly Perturbed Boundary Value Problem in Conservation Form", ibid.

[6] P.A. Markowich, C.A. Ringhofer, S. Selberherr, "A Singular Perturbation Approach for the Analysis of the Fundamental Semiconductor Equations", MRC Report £2482, Uni. of Wiscon.