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Multilevel Adaptive Methods for Semilinear Equations with Applications to Device Modelling

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1 Introduction

The drift-diffusion equations modelling the steady state electrical behaviour of a semiconductor device present several challenging problems for the numerical analyst. These equations form a 3×3 coupled elliptic system with one or more small parameters and are typically subject to mixed boundary conditions on non-smooth domains. The solutions of this system contain both interior layers and geometric boundary singularities which require appropriately graded meshes for their accurate approximation. Since these irregularities are very complex and the precise position of interior layers is quite a delicate matter ([MRS90]), it is not possible to derive suitable meshes *a priori* and a mesh refinement process based on *a posteriori* error estimation is essential for adequate resolution. A variety of approaches to adaptivity in device modelling can be found in the numerical engineering literature (e.g., [KR93, BCD92]). Much of this is based on heuristics, e.g., refinement based on doping profile. Here we derive rigorous error estimates for a reduced class of problems and a theoretically justified efficient method of implementation.

At least two difficulties have to be considered. The first is the construction of an error estimator which works well even in the presence of small parameters. The second stems from the highly nonlinear nature of the system: Each nonlinear solve requires many linear solves which form the computational core of the solution process. If a mesh is to be adaptively determined, then in principle one may be faced with solving the nonlinear system on several intermediate meshes. To reduce the cost of such a process one should in principle solve the intermediate problems up to an accuracy commensurate with the quality of those meshes, and compute accurate solutions only on the most accurate meshes.

In this paper we shall survey some recent results on the resolution of these two

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difficulties in the context of the single semilinear equation:

$$-\lambda^2\Delta u + f(u) = 0 \tag{1.1}$$

on a polygonal domain $\Omega \subset I\!R^2$ subject to mixed boundary conditions $u = g$ on $\partial\Omega_D$, $\partial u/\partial n = 0$ on $\partial\Omega_N$, where $\partial\Omega_D$ and $\partial\Omega_N$ partition $\partial\Omega$. The "Gummel iteration" for the semiconductor system can be written as sequences of such semilinear scalar problems, but including some where the second-order term $-\lambda^2\Delta u$ is replaced by a operator of the form $-\nabla.a\nabla u$, with rapidly varying coefficient function a. A detailed analysis of (1.1) is thus the first step in the design of a fully adaptive device model. In fact, in its "off" state, the electrostatic potential u of the device satisfies the equation

$$-\lambda^2\Delta u + 2\delta^2\sinh u - d = 0. \tag{1.2}$$

Here λ^2, δ^2 can both be small and the doping profile d satisfies $|d| \leq 1$ but varies in sign across interfaces interior to Ω. On the Dirichlet boundary $\partial\Omega_D$, u is required to satisfy $u = \sinh^{-1}\left(d/2\delta^2\right)$.

In this paper we present some a posteriori error estimates for (1.1) which work well under extreme parameter ranges and in the presence of geometric singularities. For the practical implementation of the refinement process we propose an inexact Newton method, related to those in [AXE93] and [XU94], which solves (1.1) by resolving the nonlinearity on a coarse mesh and then computing a sequence of corrections by solving linear problems on successively finer grids. Numerical experiments show that this method is capable of reproducing qualitative features of solutions of (1.2) (known from singular perturbation theory), by using considerably fewer linear iterations than those used in solving (1.2) to full accuracy at each refinement step. Full details of the results reviewed here are in the thesis [FER97].

2 A Posteriori Error Estimates for Semilinear Equations

Consider the problem (1.1) subject to the stated boundary conditions. Assume there exists a weak solution $u_0 \in \mathrm{L}_\infty(\Omega)$ with $\Delta u_0 \in L_\infty(\Omega)$, that f has two continuous derivatives on $I\!R$, that $g \in \mathrm{H}^{\frac{3}{2}}(\partial\Omega_D)$ and that λ is some small parameter. With these assumptions it is shown in [FER97] (using well known linear results such as [GRI92]) that $u_0 \in \mathrm{H}^{1+\alpha}(\Omega)$, where $\alpha \in (1/4, 1]$ is a fixed constant, depending purely on the interior angles of Ω at points where the boundary segments meet. It is also assumed that the Fréchet derivative of the operator in (1.1) evaluated at u_0 has a bounded inverse as an operator from $\mathrm{H}^1_{0,\partial\Omega_D}$ to $(\mathrm{H}^1)'$.

Define a shape regular triangulation $\mathcal{T}_h$ of Ω, whose union is Ω. For each triangle $T_k \in \mathcal{T}_h$ define h_k to be its diameter and let $\mathcal{E}_h$ denote the set of edges of the triangles. h_τ is defined to be the length of an edge $\tau \in \mathcal{E}_h$. If $h, \underline{h}$ are the maximum and minimum triangle diameters we require the very mild assumption that $h\log(1/\underline{h})^{\frac{1}{2}} \to 0$, as $h \to 0$. Then, for h sufficiently small, there is a finite element solution, u_h, of (1.1) which is unique in a ball centered on u_0 in H^1. Let $[\partial u_h/\partial n]_\tau$ be the difference in the normal derivative of u_h across an edge τ of a triangle. Then for constants C_1 and C_2, the H^1 and L_2 *a posteriori* error estimates may be written as:

$$\|u_0 - u_h\|_{\mathrm{H}^1} \le C_1 \left[\lambda^2 \left\{ \sum_{\tau \in \mathcal{E}_h} h_\tau^2 \left[\frac{\partial u_h}{\partial n} \right]_\tau^2 \right\}^{\frac{1}{2}} + \left\{ \sum_{T_k \in \mathcal{T}_h} \|h_k f(u_h)\|^2_{\mathrm{L}_2(T_k)} \right\}^{\frac{1}{2}} \right], \quad (2.3)$$

$$\|u_0 - u_h\|_{\mathrm{L}_2} \le C_2 \left[\left\{ \sum_{T_k \in \mathcal{T}_h} h_k^{2\alpha} \|u_0 - u_h\|^2_{\mathrm{H}^1(T_k)} \right\}^{\frac{1}{2}} + \|u_0 - u_h\|^2_{\mathrm{H}^1} \right]. \quad (2.4)$$

The estimates (2.3) and (2.4) are analogous to estimates in [VER94] and [VER96]. However, in [VER96], the loss of H^2 regularity due to reentrant corners and/or mixed boundary conditions is handled by use of a scale of W_p^1 spaces with variable p. In this work we instead use the scale $\mathrm{H}^{1+\alpha} = \mathrm{W}_2^{1+\alpha}$. Similar L_2 estimates, but assuming full H^2 regularity, are found in [EEHJ95].

Our adaptive scheme will use the L_2 *a posteriori* error estimate (2.4). In it the second term on the right hand side is estimated using (2.3) and the first term is estimated by assuming that $\|u_0 - u_h\|_{\mathrm{H}^1(T_k)}$ may be estimated by the contribution to the right hand side of (2.3) from T_k. The constants, C_1 and C_2, are estimated in [FER97] and the best theoretical bounds are of order λ^{-2} in general. However in [FER97] it is also shown heuristically that even for small λ the numerical values of C_1 and C_2 are likely to grow more slowly than this. In order to ensure that our adaptive process is robust with respect to λ we estimate C_1 and C_2 by extrapolation from computed error estimates (2.4) for each pair of successive triangulations. The computed C_1 and C_2 conform to the heuristics mentioned above. Our adaptive scheme is: Choose an initial coarse triangulation and a tolerance. Then:

- Calculate the current finite element solution to the problem.
- Calculate the *a posteriori* error estimate (2.4), after having estimated the constants C_1, C_2. (On the first refinement step these are arbitrarily chosen to be 1.)
- If the error is greater than the chosen tolerance then refine the triangulation: A triangle is refined if its contribution to the total *a posteriori* error estimate exceeds the average error over the triangles by some tolerance.
- Repeat until the tolerance is achieved.

To test the adaptive scheme consider the "off" state PN diode problem: seek u satisfying (1.2) subject to $u = \sinh^{-1}(d/2\delta^2)$ on $\partial\Omega_D$ and $\partial u/\partial n = 0$ on $\partial\Omega_N$. Here Ω is the unit square and the boundary $\partial\Omega$ is split into $\partial\Omega_D = \{0 \times [0, 1/2)\} \cup \{1 \times [0, 1]\}$ and $\partial\Omega_N = \partial\Omega \backslash \partial\Omega_D$. d in (1.2) is the piecewise constant doping profile of the device and takes a value of $+1$ in the region $\{(x, y) : x^2 + y^2 \le 0.25\}$ and -1 elsewhere. λ and δ are small parameters, which depend on various physical attributes. In this experiment λ will vary, but δ^2 is fixed at 1×10^{-7}. For this problem $u_0 \in \mathrm{H}^{1+\alpha}$, where $\alpha < 1/2$. (In the experiments we used $\alpha = 1/2$ in (2.4)).

It has been shown using singular perturbation theory, [MAR84], that the solution of this problem has a layer at the interface between $d = +1$ and $d = -1$ and the width of this layer is of order $\lambda |\log \lambda|$ as $\lambda \to 0$. To test our adaptive scheme we try to capture the correct order of λ in the width of the interior layer in the computed finite element solution as λ varies. In principle it is difficult to define where a layer "begins" and "ends". However in this case it is known that outside the layer the exact solution is "flat" and in the regions where $d = \pm 1$ it has essentially the values $u = \pm \sinh^{-1}(1/2\delta^2)$. The layer is defined to start and end when the finite element solution is bounded away from these values by a small number — here we choose 0.03. Selected results for the PN diode problem are presented in Table 1. These show that the desired order of λ is present in the computed widths. We also observe that the number of nodes needed to compute successively more severe layers does not blow up. All the experiments in this paper are obtained using a program combining the packages PETSc (Argonne National Laboratory) and Femlab (Chalmers University of Technology) and use a tolerance of 5×10^{-3} for the adaptivity.

Table 1 shows how the numerically computed width of the layer depends on λ as $\lambda \to 0+$. The theory predicts that the width is of order $\lambda \log(\lambda)$ as $\lambda \to 0+$.

λ^2	Size of initial grid	Number of refinements	Final number of nodes	Width of layer	Order of λ in width
1×10^{-4}	10×10	15	2963	0.1527	—
5×10^{-5}	10×10	12	3894	0.1111	0.92
1×10^{-5}	20×20	16	6453	0.0526	0.93
5×10^{-6}	20×20	12	3667	0.0382	0.93
1×10^{-6}	30×30	10	4166	0.0193	0.85

3 The Inexact Newton Method

The adaptive scheme described in the previous section solves, to full accuracy, a nonlinear system for each triangulation before computing error estimates and refining the grid. Since a typical refinement process can involve refining a number of triangulations, this may involve a lot of unnecessary effort. In this section we propose an adaptive scheme that considerably reduces this effort. The scheme is similar to those proposed in Xu [XU94] and Axlesson [AXE93].

Our inexact Newton method proceeds by solving the nonlinear problem, to full accuracy, on an initial coarse triangulation and then computes corrections to the calculated solution on a sequence of successively finer triangulations. These corrections involve solving one linearised problem on each of the finer triangulations.

For this adaptive procedure it is rather difficult to prove *a priori* convergence. Instead we justify the scheme theoretically *under the assumption* that a sequence of triangulations of optimal approximation power are being generated (only weak assumptions avoiding quasi-uniformity are imposed on these meshes). Under these assumptions we can prove the well-posedness and convergence of the inexact Newton method. In Section 4 we shall demonstrate, empirically, the effectiveness of the adaptive variant of this method.

Thus, for the theory, suppose that we have a sequence of shape regular triangulations

Table 2 The number of linear solves required to solve the PIN diode problem for different values of λ and δ using the two methods.

λ^2	δ^2	Linear solves for meth. of Section 2	Linear solves for inexact Newton
1×10^{-4}	1×10^{-5}	32	17
1×10^{-4}	1×10^{-7}	22	17
1×10^{-4}	1×10^{-8}	66	53
1×10^{-5}	1×10^{-4}	64	20
1×10^{-7}	1×10^{-4}	156	32
1×10^{-8}	1×10^{-4}	310	14

$\{\mathcal{T}_h^k\}$, define h^k to be the maximum diameter of the triangles in $\mathcal{T}_h^k$ and denote $\mathcal{V}_h^k$ to be the piecewise linear finite element space corresponding to $\mathcal{T}_h^k$. Consider problem (1.1). The finite element discretisation on the kth triangulation induces a map $F_h^k : \mathcal{V}_h^k \to (\mathcal{V}_h^k)'$ defined by $(F_h^k(u_h), v_h) = (\nabla u_h, \nabla v_h) + (f(u_h), v_h)$, which has the linearisation $(F_h^k)' : \mathcal{V}_h^k \to L(\mathcal{V}_h^k, (\mathcal{V}_h^k)')$ [where $L(A, B')$ denotes the set of all linear operators $A \to B'$ and B' denotes the dual space of B]. In each case $\mathcal{V}_h^k$ must be supplied with appropriate boundary conditions. Then if u_h^k is the true finite element solution on the kth triangulation, the inexact Newton scheme generates a sequence $\{\hat{u}_h^k\}$ defined by the algorithm:

1. Set $\hat{u}_h^0 = u_h^0$, the exact solution of the nonlinear finite element problem $F_h^0(u_h^0) = 0$ in $\left(\mathcal{V}_h^0\right)'$.
2. For $k = 0, 1, 2, \ldots$, iterate the two steps:
   - Solve for $\hat{e}_h^{k+1} \in \mathcal{V}_h^{k+1}$: $\left(F_h^{k+1}\right)' (\hat{u}_h^k)\ \hat{e}_h^{k+1} = -F_h^{k+1}(\hat{u}_h^k)$
   - Update $\hat{u}_h^k$: $\hat{u}_h^{k+1} = \hat{u}_h^k + \hat{e}_h^{k+1}$

Define $\Pi_h^k u_0$ to be the finite element interpolant of u_0 at the nodes of the triangulation $\mathcal{T}_h^k$. We assume, for all k, that the following approximation properties ([STW90]) hold: $\|u_0 - \Pi_h^k u_0\|_{\mathrm{H}^1} \le C h^k \|u_0\|_{\mathrm{H}^2_W}$, $\|u_0 - \Pi_h^k u_0\|_{\mathrm{L}_2} \le C (h^k)^2 \|u_0\|_{\mathrm{H}^2_W}$ and $\|u_0 - \Pi_h^k u_0\|_{\mathrm{L}_\infty} \le C (h^k)^2 \|u_0\|_{\mathcal{C}^2_W}$. Here H^2_W is a weighted H^2 Sobolev space with weight decaying sufficiently quickly near the points of singularities on the boundary, $\mathcal{C}^2_W$ is an analogous weighted $\mathcal{C}^2$-space. It is a standard result that, if h^0 is sufficiently small, the true finite element solution on the kth triangulation, u_h^k, exists and satisfies the *a priori* error estimate:

$$\|u_0 - u_h^k\|_{\mathrm{H}^1} \le C_3 h^k \|u_0\|_{\mathrm{H}^2_W}, \quad \text{for all } k, \tag{3.5}$$

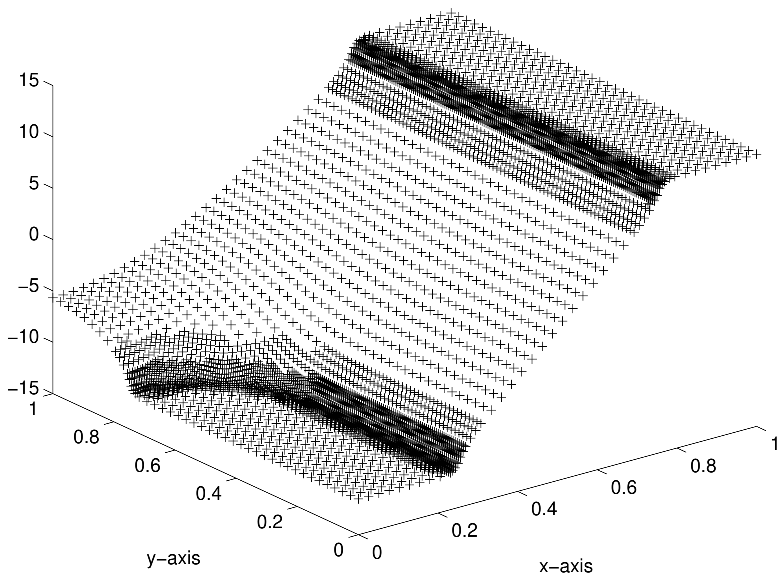
where C_3 is a constant independent of h^k and k.

In order to prove that the inexact Newton method is well-defined we need to assume that the triangulations are not too severely refined at each step. This is natural since it essentially ensures that the sequence of inexact Newton iterates stays within some suitably small ball centered on the true solution. Thus we assume that there exists a $\gamma > 0$ and $\varepsilon \in (0, 1)$, independent of h and k, such that for all k $(h^k)^2 \leq \gamma(h^0)^{1-\varepsilon} h^{k+1}$. Then it has been proved in [FER97] that, for h^0 sufficiently small, the inexact Newton solution on the kth triangulation, $\hat{u}_h^k$, is well defined for all k and satisfies the error estimate:

$$\|u_0 - \hat{u}_h^k\|_{\mathrm{H}^1} \leq C_3(1 + C_4(h^k)^{\varepsilon})h^k \|u_0\|_{\mathrm{H}^2_W}. \tag{3.6}$$

C_4 is a constant independent of h^k and k, and C_3 is the constant appearing in (3.5). Thus, neglecting higher order terms, the *a priori* error estimate for $\hat{u}_h^k$ is identical to that for u_h^k. It can also be shown that, apart from perturbations of order $(h^k)^{1+\epsilon}$, $\|u_0 - \hat{u}_h^k\|_{\mathrm{H}^1}$ is bounded above and below by $\|u_0 - u_h^k\|_{\mathrm{H}^1}$.

Figure 1 The defect correction finite element solution to the PIN diode problem when $\delta^2 = 1 \times 10^{-5}$ and $\lambda^2 = 1 \times 10^{-4}$.

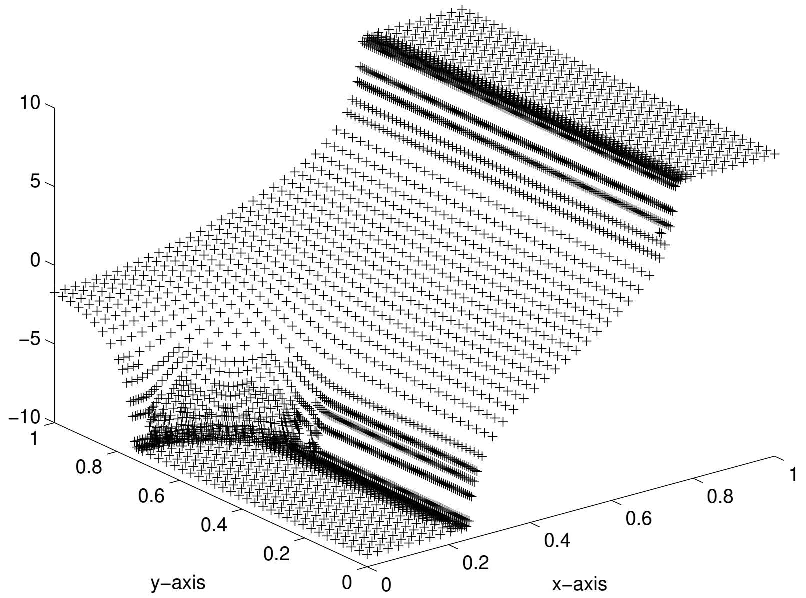


4 Experiments with the Adaptive Inexact Newton Method

The error estimates in the previous section are obtained with *a priori* determined triangulations which have optimal interpolation properties. In practice triangulations determined using adaptive L_2 refinement are used.

To test the inexact Newton method consider the PIN diode problem in its “off” state. This is a problem of the form (1.2) with the mixed boundary conditions considered in Section 2, where Ω is taken to be the unit square and $d = +1$

Figure 2 The defect correction finite element solution to the PIN diode problem when $\delta^2 = 1 \times 10^{-4}$ and $\lambda^2 = 1 \times 10^{-5}$.



in the set $\Omega_+ = \{(x,y) : 0.75 \le x \le 1,\ 0 \le y \le 1\}$, $d = -1$ in the set $\Omega_- = \{(x,y) : 0 \le x \le 0.25,\ 0 \le y \le 0.5 \text{ or } \sqrt{x^2 + (y-0.5)^2} \le 0.25\}$ and $d = 0$ in $\Omega_0 = \Omega \backslash (\overline{\Omega}_+ \cup \overline{\Omega}_-)$. The Dirichlet boundary, $\partial\Omega_D$, is the set $\{0 \times [0,1/2)\} \cup \{1 \times [0,1]\}$.

It has been shown in [MRS90] that the solution to the PIN diode problem has substantially different asymptotic behaviour in each of the cases $\lambda \ll \delta \to 0$ and $\delta \ll \lambda \to 0$. In the former case,

$$\psi|_{\Omega_+} = \sinh^{-1}\left(\frac{1}{2\delta^2}\right),\ \psi|_{\Omega_-} = \sinh^{-1}\left(\frac{-1}{2\delta^2}\right) \text{ and } \psi|_{\Omega_0} = 0,$$

whereas in the latter,

$$\psi|_{\Omega_+} = \sinh^{-1}\left(\frac{1}{2\delta^2}\right),\ \psi|_{\Omega_-} = \sinh^{-1}\left(\frac{-1}{2\delta^2}\right) \text{ and } \Delta\psi = 0 \text{ in } \Omega_0.$$

We use these known asymptotics to test the accuracy and efficiency of the adaptive inexact Newton method for a variety of λ and δ. The initial coarse triangulation was refined using the L_2 error estimate (2.4) as described in the previous section. To satisfy the conditions that the triangulations should not change too much, a maximum of 10% of the triangles were refined at each iteration and a triangle was only refined if its error estimate was twice the average of all the error estimates. Pictures of two solutions produced using the inexact adaptive Newton scheme are presented in Figures 1 and 2. These show the correct asymptotic form above (more details are in [FER97]).

The aim of the inexact Newton method is to reduce the amount of computational effort needed to find accurate finite element solutions. The method introduced in Section 2 solves a nonlinear problem for each triangulation, whereas the inexact Newton method only requires one nonlinear solve on the coarsest triangulation and then a linear solve for each of the fine triangulations. The number of linear solves required for each method for a variety of λ and δ is presented in Table 2. It was found that if the inexact Newton scheme was started with too coarse an initial triangulation or the triangles were refined too quickly then the iteration diverged. Even though the inexact Newton method may use a larger number of triangulations and nodes than the method in Section 2 [since the grids are refined more cautiously], we found that it still requires significantly fewer linear solves to produce solutions of the same accuracy.

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