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A posteriori error control in numerical simulations of semiconductor nanodevices☆

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ABSTRACT

A posteriori error estimation and control methods are proposed for a quantum corrected energy balance (QCEB) model that describes electron and hole flows in semiconductor nanodevices under the influence of electrical, diffusive, thermal, and quantum effects. The error estimation is based on the maximum norm a posteriori error estimate developed by Kopteva (2008) for singularly perturbed semilinear reaction–diffusion problems. The error estimate results in three error estimators called the first-, second-, and third-order estimators to guide the refinement process. The second-order estimator is shown to be most effective for adaptive mesh refinement. The QCEB model is scaled to a dimensionless coupled system of seven singularly perturbed semilinear PDEs with various perturbation parameters so that the estimator can be applied to each PDE on equal footing. It is found that the estimator suitable for controlling the approximation error of one PDE (one physical variable) may not be suitable for another PDE, indicating that different parameters account for different boundary or interior layer regions as illustrated by two different semiconductor devices, namely, a diode and a MOSFET. A hybrid approach to automatically choosing different PDEs for calculating the estimator in the adaptive mesh refinement process is shown to be able to control the errors of all PDEs uniformly.

1. Introduction

In order to keep pace with the increasing speed of miniaturization of modern semiconductor technology, a great variety of device models that deal with quantum effects, accuracy, robustness, and efficiency in real-life simulations have been intensively developed and tested in recent years, see e.g. [1–17] and references therein. A class of macroscopic quantum mechanical models that are based on the density-gradient (DG) theory of Ancona and Tiersten [1] has been shown to effectively simulate multi-dimensional metal oxide semiconductor field effect transistor devices (MOSFET) [18–20] with gate lengths ranging from 50 nm down to 6 nm [2,4,5,7,8,15,21,22]. The DG theory is derived from Bohm's quantum theory [23] in semiconductor context. It generalizes the equation of state for an ideal electron gas to include DG dependence and corrects the electric field by adding the Bohm potential in the drift term. The macroscopic DG models thus exhibit the essential quantum effects of nonlocality, confinement, and tunneling.

In this paper, we consider in particular the quantum corrected energy balance (QCEB) model proposed in [5] that extends the classical drift–diffusion (DD) model to include the DG quantum potential and energy balance equations in order to deal with both quantum effect and hotspot problems in nanoscale device design [24,25]. The QCEB model has been shown by Jüngel [9] as a simplified balance model that can be derived from the quantum energy transport (QET) equations based on the Chapman–Enskog expansion and Fermi–Dirac distributions. The simplification is made by assuming Maxwellian distributions, parabolic energy band structures, and the inelastic collision approximated by a Fokker–Planck ansatz [9]. For more QET models, we refer to Refs. [9,11,16,21,26].

The QCEB model consists of seven PDEs in which every PDE is self-adjoint and semilinear with respect to its unknown function. The self-adjoint form is due to the Slotboom formulation of continuity and energy balance equations. It is well known that the Slotboom formulation incurs overflow problems in computer implementation for micronscale semiconductor devices to which the applied voltage is much greater than that to nanoscale

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devices. The applied voltage is scaled down to about 1 V in nanodevices. In other words, the overflow problem is no longer a difficult issue for simulating nanodevices by self-adjoint models. Moreover, the ill-conditioning of Slotboom-type matrices in discretization can also be alleviated by suitable scalings for the matrix system [5,27]. The self-adjoint formulation provides many useful properties for the resulting nonlinear algebraic systems such as global convergence and fast linear solvers because Slotboom-type matrices are diagonally dominant M-matrices [28–30] that lead to these appealing properties [5,29–32].

We reformulate the QCEB model here to a dimensionless form of singularly perturbed system involving seven singular perturbation parameters called Debye (one), Planck (two for electrons and holes), DD (two), and EB (two) parameters. The Debye and Planck parameters are conventional parameters related to the electrostatic and quantum effects, respectively. The DD and EB parameters are associated with the diffusivity and thermal conductivity of a device in terms of the electrostatic and quasi-Fermi potentials, respectively. It is shown that the lowest order of the EB parameter is of $O(10^{-33})$ whereas that of the conventional Debye parameter is of $O(10^{-5})$. This indicates that the investigation of singularities in nanodevice models should be extended to all parameters in a model other than just one.

Across the junction between different types of semiconductors in a device or the interface of semiconductors and metal (or oxide), there are thin regions – called interior or boundary layers – of rapid variations of electrostatic and quantum potentials, charge carrier densities, or temperatures [5]. To obtain reliable approximations of layer solutions in an efficient way, one may need to use locally refined meshes that are fine in layer regions and coarse elsewhere. The refinement schemes can be categorized into two classes: *a priori* refinement using special meshes such as those of Shishkin and Bakhvalov [33,34] and *a posteriori* refinement using an adaptive algorithm that automatically generates fine meshes in layer regions starting with a simple initial mesh provided that a reliable error estimator is used to guide the refinement process [35–38]. The first class is very successful for a single PDE for which the layer region is a priori known so that the entire domain can be divided into two uniform-mesh regions, one is coarse and the other is fine. The division is determined by the perturbation parameter [34]. The resulting piecewise-uniform mesh then leads to a uniformly convergent approximation of the singularly perturbed PDE in the discrete maximum norm, i.e., the convergence is independent of the size of the singular perturbation parameter.

The adaptive mesh refinement scheme proposed in this paper belongs to the second class. The first class schemes are not suitable for the QCEB model due to the following reasons. (i) The doping junctions are curves, together with the material interfaces, that may yield overly refined piecewise-uniform meshes. (ii) The QCEB model has seven singular perturbation parameters for which it is impossible to determine a priori their strengths and locations of singularity since these parameters depend on physical conditions that may vary with devices as well as physical conditions.

A variety of a posteriori error estimators have been proposed in the literature. Most of them are based on the global error in weak energy norms for a large class of simple linear elliptic model problems [39–43]. The QCEB model consists of convection–diffusion PDEs in which the transport process dominates in junction and contact regions while the diffusion process is confined to other regions. The current state of error estimators for the convection-dominated problems is still far from satisfactory [44] because the error estimators derived from weak norms depend on an excessive power of the small diffusion parameter [45,46].

The novelty of Kopteva's estimate [33] is that it holds true uniformly in the small diffusion parameter for both boundary and interior layer solutions and is in the maximum norm, which is sufficiently strong to capture the extremely thin layer solutions of nanodevice models. Moreover, it is free of the mesh aspect ratio condition generally required by the standard finite element estimates [33,45]. We find that these properties are quite useful for the 1-irregular rectangular mesh refinement scheme used here, i.e., every finite element edge contains at most one irregular node, since the estimate is derived from finite difference (rectangular) approximation.

Three error estimators, namely, the first-, second-, and third-order estimators can be derived from Kopteva's estimate involving the first, second, and third derivative approximations of the so lution of a singularly perturbed PDE, respectively. It has been shown that the second estimator is most effective for both uniform and Bakhvalov meshes in [33], so as shown in this paper for adaptive mesh. The effectiveness is determined by the ratio of the estimator to the exact error of a constructed PDE in the maximum norm with respect to various degrees of freedom (DOFs) of meshes. The second estimator is then used to guide the refinement process in QCEB simulations on two semiconductor devices, i.e., a diode and a MOSFET. However, a device may exhibit different types of singularities in different regions where different physical properties are governed by different PDEs in a model. For example, the quantum potential of QCEB has a boundary layer near the oxide region while the hot carriers are primarily concentrated along the junction layer or near the drain contact [5]. We thus face a problem of which PDE or which singular perturbation parameter should be used to calculate the estimator during the adaptive refinement process so that the approximation errors of all PDEs in QCEB can be uniformly controlled. The main contribution of the present work is to present a new formulation of QCEB with different types of singular perturbation parameters that can be used to study various layers of state variables in a device and to uniformly control the errors of all these variables. For this, we propose a hybrid method that automatically calculates the estimator via different PDEs in QCEB during the adaptive refinement process.

The rest of the paper is organized as follows. In Section 2, we outline the QCEB model proposed in [5]. A full dimensionless formulation of the model with singular perturbation parameters is then given in Section 3. For clarity, we recall Kopteva's theorem in Section 4 and derive the three error estimators for the 1-irregular mesh refinement scheme. In Section 5, numerical results of a singularly perturbed PDE with exact solution, diode, and MOSFET are given to show the effectiveness of the second estimator, nonuniform convergence of all PDEs with the estimator fixed to one PDE, and uniform convergence with the hybrid error control method. Concluding remarks are given in Section 6.

2. A quantum energy-transport model

The QCEB model of [5] is

$$-\Delta\phi = f_1(\phi) = \frac{q}{\varepsilon}\begin{bmatrix} -n_I \exp\left(\dfrac{\phi+\phi_{qn}}{V_T}\right)\widehat{n} \\ +n_I \exp\left(\dfrac{-\phi-\phi_{qp}}{V_T}\right)\widehat{p} + C \end{bmatrix}, \tag{2.1}$$

$$-\Delta r_n = f_2(r_n) = \frac{-r_n}{2b_n}\left[V_T \ln(r_n^2) - V_T \ln(n_I\widehat{n}) - \phi\right], \tag{2.2}$$

$$-\Delta r_p = f_3(r_p) = \frac{r_p}{2b_p}\left[-V_T \ln(r_p^2) + V_T \ln(n_I\widehat{p}) - \phi\right], \tag{2.3}$$

$$-\nabla\cdot D_4(\phi)\nabla\widehat{n} = f_4(\widehat{n}) = \frac{q\left(n_{eq}p_{eq} - n_I^2\exp(\frac{\phi_{qn}-\phi_{qp}}{V_T})\widehat{n}\widehat{p}\right)}{\tau_0\begin{bmatrix} n_I\exp\left(\dfrac{\phi+\phi_{qn}}{V_T}\right)\widehat{n} + n_I\exp\left(\dfrac{-\phi-\phi_{qp}}{V_T}\right)\widehat{p} \\ +2\sqrt{n_{eq}p_{eq}}\exp\left(\dfrac{\varepsilon_t-\varepsilon_i}{k_BT_L}\right)\end{bmatrix}}, \tag{2.4}$$