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Application of the homotopy analysis method to the Poisson–Boltzmann equation for semiconductor devices

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ABSTRACT

This paper describes the application of a recently developed analytic approach known as the homotopy analysis method to derive an approximate solution to the nonlinear Poisson–Boltzmann equation for semiconductor devices. Specifically, this paper presents an analytic solution to potential distribution in a DG-MOSFET (Double Gate-Metal Oxide Semiconductor Field Effect Transistor). The DG-MOSFET represents one of the most advanced device structures in semiconductor technology and is a primary focus of modeling efforts in the semiconductor industry.

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1. Introduction

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The potential distribution in a 1-D silicon semiconductor device is described by a variant of the nonlinear Poisson–Boltzmann equation,

$$\frac{d^2\psi}{dx^2} = \frac{-q_e}{\varepsilon_s} \left[N_A e^{\frac{-\psi}{\phi_t}} - N_A - \frac{N_i^2}{N_A} e^{\frac{\psi}{\phi_t}} + \frac{N_i^2}{N_A} \right] \tag{1}$$

where ψ is the electric potential, x is distance, N_A is the doping concentration in the silicon film, N_i is the intrinsic carrier concentration, q_e is the charge of an electron, ε_s is the permitivity of silicon, and $\phi_t = kT$ is the thermal voltage where k is the Boltzmann constant and T is temperature. By applying different boundary conditions, a wide range of semiconductor devices can be modeled. This paper focuses on a large class of devices known as DG-MOSFETs (Double Gate-Metal Oxide Semiconductor Field Effect Transistors) which are described by the following boundary conditions

$\left. \frac{d\psi}{dx} \right _{x=0} = 0$	(2)
$ \lambda = 1/2$	(3)

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Two particular devices that have seen a lot of attention lately are the Symmetric DG-MOSFET [1-6] and the thin-film MOSFET on a thick insulating substrate [7-10]. The former is one of several technologies promising to extend Moore's Law [11], and the latter is of interest to the flat-panel display community. Both of these devices can be modeled by applying boundary conditions (2) and (3) to (1).

Although many specialized commercial packages are available to compute numerical solutions to (1) using finite difference or finite element techniques and generic math packages such as Mathematica can compute numeric solutions using Runge–Kutta techniques, there has been very little published on analytical techniques. In this paper, we apply an analytic solution technique, the homotopy analysis method (HAM), to the Poisson–Boltzmann equation for semiconductor devices.

Developed in 1992 by Liao [12,13], HAM is a general analytic technique for generating series solutions to various kinds of nonlinear problems in science and engineering. Many problems have already been solved using HAM including nonlinear oscillations [14–17], boundary layer flows [15,18,19], heat transfer [19,20], nonlinear water waves [17,21], the Thomas–Fermi equation [22,23], and many more. Unlike perturbation methods, the range of validity of the HAM solution is not limited to problems with small or large parameters. HAM provides a simple way to ensure the convergence of the series solution and is therefore valid for strongly nonlinear problems. Most importantly, HAM provides the freedom to choose the proper basis functions which are specific to each particular nonlinear problem. Along with the basis functions, the user of HAM must also choose other parameters and functions including the initial approximation, the auxiliary linear operator, the auxiliary function, and the auxiliary parameter. These user-specified parameters and functions will be discussed in Section 2. Although Liao provides some general rules for choosing these parameters, currently there are no specific rules governing these choices. The user must employ a "trial and error" approach in order to obtain parameters and functions that lead to a rapidly converging series solution.

2. An overview of HAM

Consider the following differential equation:

$$\mathcal{A}[u(t)] = 0 \tag{4}$$

where A is a nonlinear operator, t is the independent variable, and u(t) is the exact solution of the nonlinear differential equation. Let $u_o(t)$ be an initial approximation for u(t). HAM is based on a mapping from $u(t) \Rightarrow \Phi(t;q)$ such that as q, the so-called embedding parameter, goes from 0 to 1, $\Phi(t;q)$ varies from the initial guess $u_o(t)$ to the exact solution u(t). This mapping is generated by the *zero-order deformation equation* which is expressed as

$$(1-q)\mathcal{L}[\Phi(t;q) - u_o(t)] = qhH(t)\mathcal{A}[\Phi(t;q)]$$
(5)

where $\Phi(t;q)$ is subject to the initial boundary conditions and where $h \neq 0$ is the auxiliary parameter, $H(t) \neq 0$ is the auxiliary function, and \mathcal{L} is the auxiliary linear operator.

First of all, it is assumed that \hbar , H(t), $u_o(t)$, and \mathcal{L} are chosen such that the solution $\Phi(t;q)$ to the zero-order deformation equation exists as do all derivatives with respect to q. Then defining

$$u_{o}^{[k]}(t) \equiv \frac{\partial^{k} \Phi(t;q)}{\partial q^{k}} \bigg|_{q=0}$$
(6)

where $u_0^{[k]}$ is called the *kth-order deformation derivative* and

$$u_k(t) \equiv \frac{1}{k!} \left. \frac{\partial^k \Phi(t;q)}{\partial q^k} \right|_{q=0} = \frac{1}{k!} \left. u_o^{[k]}(t),$$
(7)

 $\Phi(t;q)$ can be expanded in a power series in q

$$\Phi(t;q) = \Phi(t;0) + \sum_{k=1}^{\infty} \frac{1}{k!} \frac{\partial^k \Phi(t;q)}{\partial q^k} \bigg|_{q=0} q^k$$
(8)

or

$$\Phi(t;q) = u_o(t) + \sum_{k=1}^{\infty} u_k(t)q^k.$$
(9)

From (9) it can be seen that when q = 1 then

$$u(t) = u_o(t) + \sum_{k=1}^{\infty} u_k(t)$$
(10)

where $u_o(t)$ satisfies the stated boundary conditions and each $u_k(t)$ has zero boundary values. The *K*th order HAM approximation of u(t) is given by

$$u(t) \approx \sum_{k=0}^{K} u_k(t).$$
(11)

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