ESSENTIALLY NON-OSCILLATORY METHODS FOR TWO-DIMENSIONAL HYDRODYNAMIC MODELS

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ABSTRACT

A one carrier, two dimensional MESFET device of the size $0.6 \times 0.2\mu m^2$ is simulated using the hydrodynamic model and a third order Essentially Non-Oscillatory (ENO) finite difference method. The effect of boundary conditions is shown by varying the types of boundary conditions. ENO is observed stable under most boundary conditions including the over-specified ones, which produce boundary layers at various locations. The grid used is coarse (96×32) and a jump of many magnitudes in the concentration due to the doping and the boundary condition at the gate can be handled well. A resolution study is also performed by refining the grid. The result indicates the potential of the ENO method as an inexpensive (due to the coarse grid it can use) and robust tool for multi-dimensional device simulations.

1 Introduction

Essentially Non-Oscillatory (ENO) finite difference methods are high order non-linearly stable methods suitable for solving problems with shocks or high gradient regions. One dimensional device simulation using ENO schemes was first performed in [1]. In this work we are interested in 2D simulations. We use the ENO schemes based on point values and TVD high order Runge-Kutta time discretizations of Shu and Osher [3], [4], [5], which has the advantage of simplicity and cost-effectiveness for 2D and 3D. For this purpose the hydrodynamic (HD) model in device simulation is written as a conservation law plus forcing terms for the momentum and energy equations, and dissipation terms for the energy equation. The similarity between the HD model and compressible Navier-Stokes equations in gas dynamics makes the adapting of ENO schemes possible.

A one carrier, two dimensional MESFET device of the size $0.6 \times 0.2\mu m^2$ is simulated. One special case of ENO simulation on this device is reported by us in [2], which also contains more technical details than this paper. We observe stable solutions which exhibit complicated structures including high gradient regions. In this paper the effect of boundary conditions is shown by varying the types of boundary conditions. ENO is observed stable under most boundary conditions including the over-specified ones, which make boundary layers at various locations. The grid used is coarse (96×32) and a jump of many magnitudes in the concentration due to the doping and the boundary condition at the gate can be handled well. The result indicates the potential of the ENO method as an inexpensive (due to the coarse grid it can use) and robust tool for multi-dimensional device simulations. The ENO method is applicable to any device model which can be written into a hyperbolic conservation law plus forcing terms and viscosities.

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2 ENO Scheme and the HD Model in Conservation Form

We shall only sketch ENO schemes here. More details can be found in [3], [4] and [5]. ENO is a method to solve a system of hyperbolic conservation laws of the form $u_t + \sum_{i=1}^{d} f_i(u)_{x_i} = g(u,x,t)$, where $u = (u_1, \cdots, u_m)^T$ is a vector and $\sum_{i=1}^{d} \xi_i \frac{\partial f_i}{\partial u}$ is diagonalizable with real eigenvalues for any real $\xi = (\xi_1, \cdots, \xi_d)$. Initial or initial-boundary conditions are added. Local field by field decomposition is used, to resolve waves in different characteristic directions. The multidimensional cases are treated dimension by dimension: when computing $f_i(u)_{x_i}$ in any particular direction, variables in all other directions are kept constant. This, in essence, reduces the determination of the scheme to the case of a single conservation law in one spatial dimension. The conservative high order approximation to this single derivative is achieved by polynomial interpolations with an adaptive stencil trying to automatically choose a local smoothest stencil in the presence of discontinuities. Steady states are reached by explicit time stepping using the TVD (total-variation-diminishing) high order Runge-Kutta methods in [3]. The computer program is fully vectorized for computations on Cray supercomputers. For details of the efficient implementation, see [5].

The hydrodynamic model is written into a conservation laws format by defining the vector $u = (n, \sigma, \tau, W)$, where n is the concentration, $p = (\sigma, \tau)$ is the momentum, and W is the total energy. The HD model then becomes

$$u_t + f_1(u)_x + f_2(u)_y = c(u) + G(u,\phi) + (0,0,0,\nabla\cdot(\kappa\nabla T)), \tag{2.1}$$

with

$$f_1(u) = (\frac{\sigma}{m}, \frac{2}{3}(\frac{\sigma^2}{mn} + W - \frac{\tau^2}{2mn}), \frac{\sigma\tau}{mn}, \frac{5\sigma W}{3mn} - \sigma\frac{\sigma^2+\tau^2}{3m^2n^2}), \tag{2.2}$$

$$f_2(u) = (\frac{\tau}{m}, \frac{\sigma\tau}{mn}, \frac{2}{3}(\frac{\tau^2}{mn} + W - \frac{\sigma^2}{2mn}), \frac{5\tau W}{3mn} - \tau\frac{\sigma^2+\tau^2}{3m^2n^2}), \tag{2.3}$$

$$c(u) = (0, -\frac{\sigma}{\tau_p}, -\frac{\tau}{\tau_p}, -\frac{W - W_0}{\tau_w}), \qquad G(u) = (0, -enF_1, -enF_2, -enF\cdot v), \tag{2.4}$$

where m is the effective electron mass, τ_p and τ_w are the momentum and energy relaxation times, W_0 is the constant rest energy, e is the electron charge modulus, v is the velocity, and $F = -\nabla\phi$ is the electric field obtained from the coupled Poisson equation: $\nabla\cdot(\epsilon\nabla\phi) = -e(n - n_d)$, where n_d is the doping and ϵ is the dielectric constant.

3 Numerical Simulation Results

We now present numerical simulation results for a one carrier, two dimensional MESFET device. The hyperbolic part is approximated by ENO, and the Poisson equation is solved by central differencing using Successive Over-Relaxation (SOR) or the Conjugate Gradient (CG) method. A continuation method is used to reach the steady state: the voltage bias is taken initially as zero and is gradually increased to the required value, with the steady state solution of a lower biased case used as the initial condition for a higher one. The two dimensional MESFET we simulate is of the size $0.6 \times 0.2\mu m^2$. The source and the drain each occupies $0.1\mu m$ at the upper left and the upper right, respectively, with the gate occupying $0.2\mu m$ at the upper middle (Figure 1, left). The doping is defined by $n_d = 3 \times 10^{17} cm^{-3}$ in $[0,0.1] \times [0.15,0.2]$ and in $[0.5,0.6] \times [0.15,0.2]$, and $n_d = 1 \times 10^{17} cm^{-3}$ elsewhere, with abrupt junctions (Figure 1, right). A uniform grid of 96×32 points is used, and a resolution study using 192×64 points is performed. Notice that even if we may not have shocks in the solution, the initial condition $n = n_d$ is discontinuous, and the final steady state solution has a sharp transition around the junction. With the relatively coarse grid we

use, the non-oscillatory shock capturing feature of the ENO algorithm is essential for the stability of the numerical procedure.

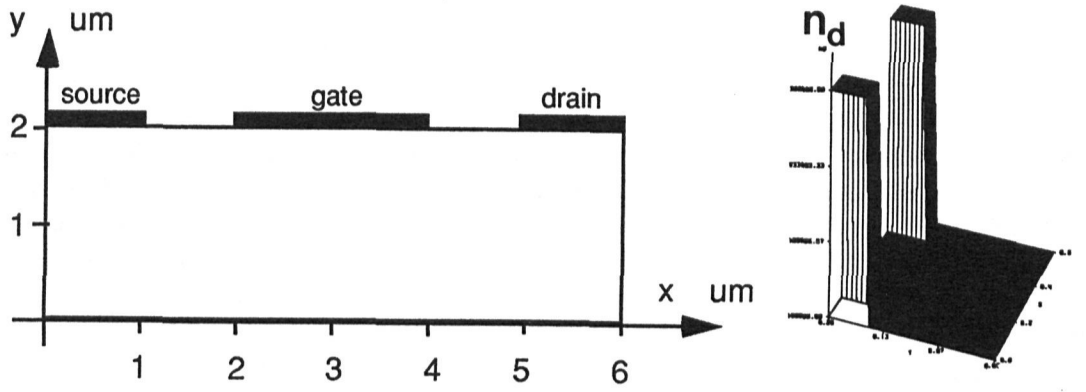

Figure 1: Two dimensional MESFET. Left: the geometry; Right: the doping n_d

We apply, at the source and drain, a voltage bias $vbias = 2V$. The gate is a Schottky contact, with a negative voltage bias, $vgate = -0.8V$ and a very low concentration value, $n = 3.9 \times 10^5 cm^{-3}$. The lattice temperature is taken as $T_0 = 300°K$.

The numerical boundary conditions used in [2] are as follows: at contacts (source, gate and drain), potential Φ, concentration $n = n_d$, temperature $T = T_0$ and tangential velocity $u = 0$ are prescribed; normal velocity v at contacts and all variables at other parts of the boundary are equipped with Neumann boundary conditions. In Figure 2, we show pictures of the concentration n (top) and the temperature T (bottom). Surfaces of the solution are shown at the left, and cuts at $y = 0.175$, which cut through the middle of the high doping "blobs" horizontally, are shown at the right (plus symbols). In order to verify the resolution of the ENO scheme on this relatively coarse grid, we have also computed the same problem doubling the number of grid points in each direction (192×64 points). The result is shown as solid lines in the cuts.

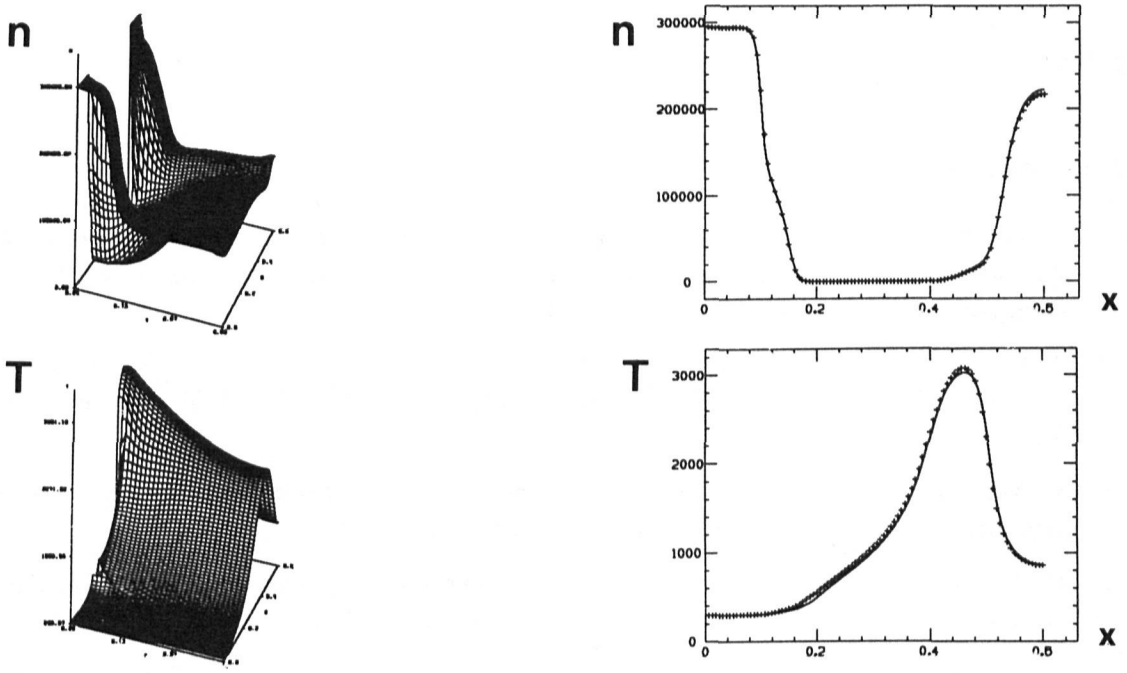

Figure 2: Two dimensional MESFET, concentration n (top) and temperature T (bottom). Left: surface of the solution; Right: cut at $y = 0.175$ (plus: 96×32 points; solid line: 192×64 points).

Notice that there is a boundary layer for the concentration n at the drain, but not at the source. Also notice the rapid drop of n at the depletion region near the gate. The temperature achieves its maximum around the left corner of the drain.

The boundary conditions chosen are based upon physical and numerical considerations. They may not be adequate mathematically, as is evident from some serious boundary layers observable in Figure 2. ENO methods, owing to their upwind nature, are robust to different boundary conditions (including over-specified boundary conditions) and do not exhibit numerical difficulties in the presence of such boundary layers, even with the extremely low concentration prescribed at the gate (around 10^{-12} relative to the high doping). We point out, however, that boundary conditions affect the global solution significantly. In Figure 3, we show the simulation results for the temperature T with two different sets of boundary conditions: Dirichlet boundary conditions everywhere for the temperature $T = T_0$ (left), and Neumann boundary conditions for all variables except for the potential at the contacts (right). This should be compared with Figure 2. Apparently there are noticeable differences. This indicates the importance of studying adequate boundary conditions, from both a physical and a mathematical point of view.

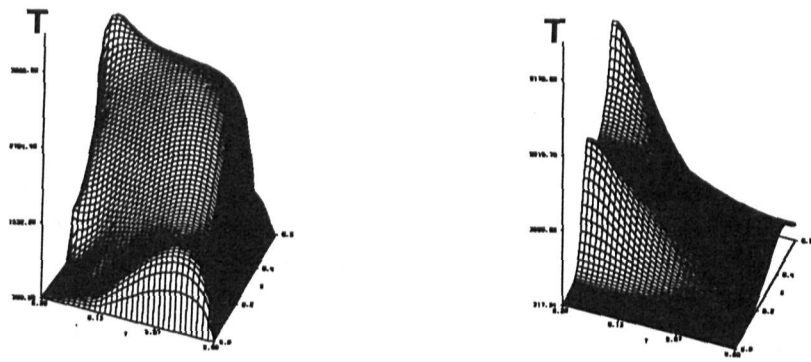

Figure 3: Two dimensional MESFET, temperature T. Surface of the solution. Left: Dirichlet boundary condition for T; Right: Neumann boundary conditions for all variables except the potential at the contacts.

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