Analysis and Simulation of Extended Hydrodynamic Models: The Multi-Valley Gunn Oscillator and MESFET Symmetries

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We introduce a novel two carrier hydrodynamic model, which incorporates higher dimensional geometric effects into a one dimensional model. We study (1) the GaAs device in the notched oscillator circuit, and, (2) a MESFET channel, and its symmetries. We present new mathematical results for a reduced model.

Keywords: Gunn oscillator, Two carrier hydrodynamic model, MESFET, symmetry, geometric structure terms

1. INTRODUCTION

In previous work, we have demonstrated the robustness of an algorithm (ENO: Essentially Non-Oscillatory) designed for the simulation of the hydrodynamic model for semiconductors over a wide range of parameters. In [8] and [9], $n^+ - n - n^+$ diodes in one dimension and MESFETS in two dimensions were simulated. Here we allow multi-species and geometric source terms.

1.1. Description of the Gunn Oscillator

The equations describing an RLC tank circuit, connected to a Gunn oscillator, are:

$$V_D(t) = V_B - L \frac{dI(t)}{dt}, \quad I(t) = I_d(t) + C \frac{dV_D(t)}{dt} + \frac{V_D(t)}{R}, \quad (1.1)$$

where $V_D(t)$ is the voltage at the device terminal, V_B is the bias voltage, $I(t)$ is the current flowing through the battery, and C is the total capacitance, which includes the so-called cold capacitance. $I_d(t)$ is the particle current. In [10], a Monte-Carlo simulation of the Boltzmann equation was used to update $I_d(t)$. Earlier, a single valley hydrodynamic model was used by [6], whereas here we employ a two-valley hydrodynamic model. The coupling terms and the system have the structure of [1].

1.2. Basic MESFET Description

Next we describe a two dimensional MESFET of the size $0.6 \times 0.2 \mu\text{m}^2$. The source and the drain each occupies $0.1 \mu\text{m}$ at the upper left and the upper right, respectively, with a gate occupying $0.2 \mu\text{m}$ at the upper middle (Fig. 1, left). The doping is defined by $n_d = 3 \times 10^5 \mu\text{m}^{-3}$ in $[0, 0.1] \times [0.15, 0.2]$ and in $[0.5, 0.6] \times [0.15, 0.2]$, and $n_d = 1 \times 10^5 \mu\text{m}^{-3}$ else-

FIGURE 1 Two dimensional MESFET. Left : the geometry and the doping n_d ; right: the contour of the concentration n when $vbias = 2.0V$ and $vgate = -0.8V$

where. We apply, at the drain, voltage biases varying up to $vbias = 2V$. The gate is a Schottky contact, with negative voltage bias up to $vgate = -0.8V$ and very low concentration value $n = 3.8503 \times 10^{-8} \mu m^{-3}$ (following Selberherr [12]). The lattice temperature is taken as $T_0 = 300 K$.

In Fig. 1, right, we show the contour of the concentration n when $vbias = 2V$ and $vgate = -0.8V$. We can see an approximate spherical symmetry around the upper middle point. This serves as a basis for our reduced 1D model with spherically symmetric forcing terms in the next two sections. The velocity v also shows a similar spherical symmetry. However, temperature T and potential Φ do not reveal spherical symmetry at this $vbias$.

2. MATHEMATICAL RESULTS : A WELL POSED REDUCED MODEL

Consider a reduced model, the compressible, two carrier, Euler-Poisson equations :

$$\begin{aligned} \partial_t \rho_i + \nabla \cdot \vec{m}_i &= R_i(\rho_1, \rho_2), \\ \partial_t \vec{m}_i + \nabla \cdot \left(\frac{\vec{m}_i \otimes \vec{m}_i}{\rho_i} \right) + \nabla p(\rho_i) &= \rho_i \nabla \phi - \frac{\vec{m}_i}{\tau_i} + \vec{H}_i(\rho_1, \rho_2, E_1, E_2), \\ \Delta \phi &= \rho_1 + \rho_2 - n_d(\vec{x}), \quad i = 1, 2, \quad \vec{x} \in \mathbf{R}^N, \end{aligned} \quad (2.2)$$

where $\rho_i(\vec{x}, t)$, $\vec{m}_i(\vec{x}, t)$, and $\phi(\vec{x}, t)$ denote the density, the momentum, and the potential of the flows, respectively, and $p(\rho_i) = \rho_i^\gamma / \gamma$, $\gamma > 1$, is the pressure, $E_i = \frac{\rho_i^{\gamma-1}}{\gamma(\gamma-1)} + \frac{|\vec{m}_i|^2}{2\rho_i^2}$ the mechanical energy,

$\tau_i > 0$ is the momentum relaxation time, and $n_d(\vec{x})$ is the doping profile. The initial-boundary problem for the system (2.2) with geometrical symmetry is :

$$\begin{aligned} \partial_t \rho_i + \partial_x m_i &= a(x) m_i + R_i(\rho_1, \rho_2), \\ \partial_t m_i + \partial_x \left(\frac{m_i^2}{\rho_i} + p(\rho_i) \right) &= a(x) \frac{m_i^2}{\rho_i} + \rho_i \phi_x - \frac{m_i}{\tau_i} + H_i(\rho_1, \rho_2, E_1, E_2), \\ \phi_{xx} &= a(x) \phi_x + \rho_1 + \rho_2 - n_d(x), \quad i = 1, 2, \end{aligned} \quad (2.3)$$

$$\begin{aligned} (\rho_i, m_i) |_{t=0} &= (\rho_{i0}(x), m_{i0}(x)), \\ m_i |_{x=1} &= m_i |_{x=2} = 0, \\ \phi |_{x=1} &= \phi_1(t) \in \mathbf{L}^\infty, \quad \phi |_{x=2} = \phi_2(t) \in \mathbf{L}^\infty, \end{aligned} \quad (2.4)$$

where the field term ϕ_x is nonlocal (self-consistent) and $a(x)$ is a C^1 function that can be represented by $a(x) = -A'(x)/A(x)$. The function $A(x)$ describes the cross-sectional area at x in a variable-area duct such as a nozzle channel, and $A(x) = \frac{2\pi^{N/2}}{\Gamma(N/2)} x^{N-1}$ for spherically symmetric flow in N dimensions, such as

in the MESFET, for the one carrier case we test in the next section.

The Euler-Poisson equations for two carriers with $a(x) = 0$ have been studied for some special couplings: The case $R_i = H_i = 0$ in [11] by the Godunov scheme with fractional step techniques and the case $R_i = (1 - \rho_1 \rho_2) Q(\rho_1, \rho_2)$, $H_i = 0$, $0 \leq Q(\rho_1, \rho_2) \leq \frac{Q_0}{1 + \rho_1 + \rho_2}$ in [7] by the viscosity method. The system

for one carrier with general $a(x) \in C^1$ is solved in [5].

We develop a new shock capturing numerical scheme and apply this scheme to construct global entropy solutions to the system (2.3-2.4) with nonzero $a(x)$ and general R_i and H_i . More precisely, we consider the following coupling terms $R_i(\rho_1, \rho_2)$ and $H_i(\rho_1, \rho_2, E_1, E_2)$:

(A1) R_i and H_i are Lipschitz functions in the variables $\rho_1 \geq 0$, $\rho_2 \geq 0$, E_1 , and E_2 .

(A2) There exist a constant $C > 0$ and a decomposition of R_i : $R_i(\rho_1, \rho_2) = R_i^+(\rho_1, \rho_2) - R_i^-(\rho_1, \rho_2)$ with $R_i^\pm(\rho_1, \rho_2) \geq 0$ such that, for all $\rho_1, \rho_2 > 0$ and $i = 1, 2$,

$$\begin{aligned} R_i(\rho_1, \rho_2) &\leq C, & |H_i(\rho_1, \rho_2, E_1, E_2)| &\leq C\rho_i; \\ \text{When } R_i^+(\rho_1, \rho_2) &\geq R_i^-(\rho_1, \rho_2) & \text{and } \rho_i &\geq (\theta/(\theta+1))^{1/\theta}, \\ & & R_i^+(\rho_1, \rho_2) &\leq C\rho_i; \\ \text{When } R_i^+(\rho_1, \rho_2) &< R_i^-(\rho_1, \rho_2), & 0 < R_i^-(\rho_1, \rho_2) &\leq C\rho_i. \end{aligned}$$

Theorem 2.1 *Let $a(x)$ be a C^1 function and $1 < \gamma \leq 5/3$. Let $R_i(\rho_1, \rho_2)$ and $H_i(\rho_1, \rho_2, E_1, E_2)$ satisfy Assumptions (A1)–(A2). Then there exists a sequence of approximate solutions $(\rho_i^h(x, t), m_i^h(x, t))$, for $i = 1, 2$, converging a.e. to an entropy solution $(\rho_i(x, t), m_i(x, t))$, of (2.3-2.4) such that $0 \leq \rho_i(x, t) \leq C(T) < \infty$, $|m_i(x, t)/\rho_i(x, t)| \leq C(T) < \infty$, for $0 \leq t \leq T < \infty$, $x \in \mathbf{R}$, a.e.*

Assumptions (A1)–(A2) are in fact quite general.

For example, $R_i = 0$, $R_i = \frac{1 - \rho_1 \rho_2}{1 + \rho_1 + \rho_2}$,

$R_i = \frac{(-1)^i(\rho_1 - \rho_2)}{1 + \rho_1 + \rho_2}$, $H_i = 0$, and $H_i = \frac{\rho_i E_i}{1 + E_1 + E_2}$ are

in this class. Since $a(x)$ is a nonzero function, the nonlinear resonance between characteristic modes and

geometrical source mode occurs at the sonic state, which causes extra difficulties (cf. [3]). Due to the geometrical source terms, we adopt the approach of [3]. Thus, we use the piecewise steady-state solutions, which incorporate such source terms, to replace the piecewise constants from the Riemann solutions as the building blocks. Due to the nonlocal source term, we also incorporate the fractional step procedure into our construction of approximate solutions, with the steady-state solutions as their fundamental building blocks. To obtain a uniform bound for the approximate solutions, we estimate the Riemann invariants involving the nonlocal term with the aid of the conservation of mass and the estimates of the approximate steady-state solutions and Riemann solutions. The H^{-1} compactness of the weak entropy dissipation measures can be achieved as in [2], [3]. These requirements enable us to deduce the strong convergence of the approximate solutions with the aid of a compactness framework (see [2]), proved by DiPerna

(1983) for $\gamma = 1 + \frac{2}{2s+1}$, $s \geq 2$ an integer, and by

Ding-Chen-Luo (1987) and Chen (1988) for the general case $1 < \gamma \leq 5/3$.

In [4] we consider the one-dimensional Euler-Poisson equations. It is proved that the relaxation terms prevent the development of shock waves for the smooth initial data with small oscillation, which is not true for large initial data. The nonlinear singular limit of the smooth solution to the drift-diffusion equation is shown when the relaxation times tend to zero.

3. SIMULATION RESULTS

We first present simulation results for the Gunn oscillator defined in Section 1.1. Notice that this involves solving a time dependent equation system with strong hyperbolic components, hence upwinding and high order accuracy in space and time are important, justifying the usage of ENO schemes [9]. In Fig. 2, left, we show the time history of the applied voltage $V_D(t)$. We can see sustained oscillations of a slow frequency on top of a fast frequency. In Fig. 2 right, we show the

FIGURE 2 Gunn oscillator. Left: the time history of $V_D(t)$; right: the concentration n of the first carrier at 4 equally spaced “snaps” over one period of the oscillation

concentration n of the first carrier at 4 equally spaced “snaps” over one period of the oscillation. We can see the movement of the structure clearly in such a period.

Next, we show the result of attempting to use the 1D model with a spherical symmetry assumption, to approximate the 2D MESFET described in Section 1.2. We take our 1D domain to be from $r = 0.025$ to $r = 0.1$, measured from the top middle point at $(x, y) = (0.3, 0.2)$ downwards. The boundary conditions for the concentration n , the temperature T and the potential ϕ are prescribed, using the values of the 2D simulations; the boundary condition for the velocity is floating (Neumann). In Fig. 3, left, we show the comparison, for the concentration n , of the 2D MES-

FET result with the 1D model assuming spherical symmetry, at $v_{bias} = 2.0V$ and $v_{gate} = -0.8V$. We can see a qualitatively correct agreement (the agreement is even better for lower bias). This is good since it means that other quantities (such as T and Φ) which are not spherically symmetric have minimal effect on the concentration through the nonlinear coupling of the equations. In Fig. 3, right, we show the same comparison for the temperature T . We can see that now the 1D model disagrees with the 2D results to a much greater extent, manifesting the fact that T is not spherically symmetric. If n is the only quantity of interest, then the 1D model can be used, saving substantial computing time in the simulation. Otherwise, a better model (perhaps a hybrid one with the non-symmetric

FIGURE 3 The 1D model with spherical symmetry assumption, in comparison with the 2D MESFET results. Left: the concentration n ; right: the temperature T

components computed by the 2D model and symmetric quantities computed by the 1D model) might be useful. This is currently under investigation.

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