AN ANALYSIS OF THE TIME-DEPENDENT HYDRODYNAMIC DEVICE EQUATIONS

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Abstract

A mathematical analysis of the hydrodynamic semiconductor device equations is developed using characteristic variable transformations. This theoretical treatment of the transport equations uses the eigenvalue structure of the associated flux Jacobian matrices to construct local projections from the characteristic variables to enforce boundary conditions on the primary solution variables. The one-dimensional hydrodynamic model with both parabolic and nonparabolic energy band structure is first analyzed and the implications for discrete solution approximations are discussed. The analysis is then extended to the two-dimensional case. Some aspects of the implementation for different (subcritical and supercritical) transport situations and the associated boundary conditions are also addressed.

1 Introduction

In the present work we summarize the methodology and results obtained from a recent analysis of representative parabolic and nonparabolic energy band models for the hydrodynamic device equations. The details of the study are not presented here due to space limitations, and may be found in our poster. We also consider the related problem of specifying absorbing boundary conditions that are consistent with the local type of the system of hydrodynamic device PDE's at artificial boundaries. The approach of characteristic transformations is used to define appropriate local projections for the boundary conditions. These in turn lead to a well-posed problem and a discrete model with approximately non-reflecting boundary conditions. Both subcritical and supercritical transport situations are considered. We first consider the one-dimensional problem under both parabolic and non-parabolic energy band assumptions. The heat flux term, formally an unknown which must be determined from higher-order moments of the Boltzmann equation, is neglected in our analysis under the assumption that its diffusive effect on the average energy is small at the boundaries. Typically, if not neglected, it is treated phenomenologically in existing models via a Fourier law. Lundstom [5] discusses various methods of treating the heat flux term. Gardner [1] has shown that the mathematical classification of the resulting PDE system may be affected by the choice of heat flux model. We then extend our one-dimensional analysis to the two-dimensional hydrodynamic model. Some comments on the implementation in numerical schemes are given, and a remark on the three-dimensional extension concludes the treatment.

2 Analysis

We begin with the divergence form of the one-dimensional transport equations

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{E}(\mathbf{U})}{\partial x} = \mathbf{S}(\mathbf{U}) \tag{1}$$

All we require is that $\mathbf{E(U)}$ and $\mathbf{S(U)}$ may in general be nonlinear functions of $\mathbf{U}$, but not of its derivatives. Using the chain rule for the convective flux term in (1),

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{A(U)}\frac{\partial \mathbf{U}}{\partial x} = \mathbf{S(U)}, \tag{2}$$

where $\mathbf{A(U)} \equiv \frac{\partial \mathbf{E(U)}}{\partial \mathbf{U}}$.

Our treatment of the system (2) follows the theory described by Witham [6], and serves to motivate the higher-dimensional case. First, (2) is a first order, quasilinear system of partial differential equations. Second, by definition, (2) is hyperbolic if $\mathbf{A}$ has real eigenvalues, as well as a complete set of linearly independent eigenvectors (*e.g.*, see [4]).

Besides determining the classification and behavior of the system (2), or equivalently, (1), the eigenvalues of the Jacobian matrix $\mathbf{A}$ also determine the characteristic curves. In turn, the characteristic curves determine the directions along which waves propagate through the domain. Let the characteristic curves be regarded as parameterized in time, and let the eigenvalues be denoted $\lambda_k, k = 1,2,3$. Then the characteristic trajectories are defined as the solution of the associated characteristic ordinary differential equations $\frac{dx}{dt} = \lambda_k$. It follows that the eigenvalues of the system correspond physically to the propagation speeds of each wave, and since the eigenvalues of $\mathbf{A(U)}$ are functions of the state variables, they will, in general, vary through space and time.

Next, we seek a change of dependent variables from $\mathbf{U}$ to $\hat{\mathbf{U}}$ such that $\frac{\partial \mathbf{U}}{\partial t} = \frac{\partial \mathbf{U}}{\partial \hat{\mathbf{U}}}\frac{\partial \hat{\mathbf{U}}}{\partial t}$. Let $\mathbf{T} \equiv \frac{\partial \mathbf{U}}{\partial \hat{\mathbf{U}}}$. Then $\frac{\partial \mathbf{U}}{\partial t} = \mathbf{T}\frac{\partial \hat{\mathbf{U}}}{\partial t}$. If $\mathbf{T}$ is invertible, we may solve for the partial derivative of the new variable, $\frac{\partial \hat{\mathbf{U}}}{\partial t} = \mathbf{T^{-1}}\frac{\partial \mathbf{U}}{\partial t}$.

If the matrix T is a modal matrix whose columns are the eigenvectors of $\mathbf{A}$, then it can be shown that the differential operator may be decoupled. If the system (2) is hyperbolic, then the matrix $\mathbf{T}$ has linearly independent columns, and is therefore invertible. Furthermore, the left eigenvectors of $\mathbf{A}$ are the rows of $\mathbf{T^{-1}}$, so that the product $\mathbf{T^{-1}AT}$ is a a similarity transformation on the matrix $\mathbf{A}$. The result is therefore a diagonal matrix, and the differential operator is decoupled. The component of this system associated with the k^{th} eigenvalue is

$$\frac{\partial \hat{U}_k}{\partial t} + \lambda_k \frac{\partial \hat{U}_k}{\partial x} = \hat{S}_k. \tag{3}$$

Finally, the transport equations take on a particularly simple form if one notes that the left hand side of (3) is the total derivative of $\hat{U}_k$ along a characteristic trajectory $x = x(t)$ with associated wave speed λ_k. These trajectories are exactly the characteristic curves defined above. Hence, the characteristics form of the transport equations can be written

$$\frac{D\hat{U}_k}{Dt} = \hat{S}_k \text{ on } \frac{dx}{dt} = \lambda_k, \text{ k=1,2,3.} \tag{4}$$

At this point, one could discretise (4) directly and thereby construct a solution locally, by the classical method of characteristics, *i.e.*, solving locally for the characteristic curves and advancing the solution incrementally along the characteristics. This need not be done in practice, but such an exercise is fruitful when one is considering questions such as the correct number of boundary conditions and the domain of dependence. The details of such a construction are well known, and may be found, for example, in [6]. From the persepctive of the present study, an important result is that *the number of boundary conditions applied at inflow and outflow boundaries should be equal to the number of characteristics pointing into the region.* Furthermore, in order for the problem to be

well-posed, the boundary conditions should not determine the Riemann variables which correspond to outgoing characteristics.

The multidimensional case may be handled by the same approach, although it is no longer possible to decouple the differential operator. The flux Jacobian associated with a directional derivative of the flux vector locally orthogonal to the boundary may be used to obtain the matrix T required for the projections.

3 Implementing The Boundary Conditions

A procedure for implementing the boundary conditions for the two-dimensional problem in a numerical scheme is as follows: the left eigenvectors are used to separate the flow variables into incoming and outgoing waves. Next, those quantities corresponding to incoming waves are specified explicitly as boundary data, and those quantities corresponding to outgoing waves evolve from the interior PDE solution. Finally, the corrections to the state vector are obtained from the right eigenvectors of the flux Jacobian. Let the correction to the state vector that is predicted by the numerical solver be denoted $\delta \mathbf{U_p}$. Then, the specified change in the kth Riemann variable is

$$\delta \hat{U}_{sk} = \begin{cases} 0 & \text{if } \lambda_k < 0 \\ \mathbf{l_k} \cdot \delta \mathbf{U_p} & \text{if } \lambda_k > 0 \end{cases} \tag{5}$$

Finally, the correction to the state vector for boundary condition specification to be applied through the next time step at an inflow or outflow boundary is given by applying the modal matrix T:

$$\delta \mathbf{U_s} = \mathbf{T} \delta \hat{\mathbf{U}}_\mathbf{s}, \tag{6}$$

where T is the modal matrix of the flux Jacobian and (6) is evaluated at the boundary in question.

In summary, there are the following four cases, illustrated here for the two-dimensional case:

Supercritical Outflow: All eigenvalues are positive. No boundary conditions are specified.

Supercritical Inflow: All eigenvalues are negative. Hence $\delta \hat{\mathbf{U}}_\mathbf{s} = \mathbf{0}$ so that $\delta \mathbf{U_s} = \mathbf{0}$, and all components of U are specifiedby the problem data.

Subcritical Outflow: Only one eigenvalue is negative. Therefore only one piece of information should be specified.

Subcritical Inflow: Three eigenvalues are negative. Thus three pieces of information should be specified.

4 Concluding Remarks

We have performed an eigenvalue analysis of the quasilinear, first order, time dependent systems of partial differential equations which assert the continuity of carrier mass, average momentum, and average energy. Our results show that in the special case of parabolic energy bands, the assumption of negligible drift kinetic energy is sufficient to change the mathematical classification of the system. If this assumption is made, the eigenvalues of the system become complex: there are no real characteristics. Conversely, retaining the drift kinetic energy results in a system of equations that is hyperbolic in time. The method of characteristics can then be brought to bear on the problem of specifying appropriate boundary conditions. Furthermore, we have obtained

absorbing boundary conditions that can be applied at boundaries that are artificial in the sense that they must be introduced solely to facilitate a device simulation. Finally, we have shown that a particular nonparabolic energy band model recently proposed is not hyperbolic in time. We suspect that the reason for this is that the drift kinetic energy is neglected, because this approximation has a similar effect on the parabolic band model.

In the computational fluid dynamics community, the use of absorbing boundary conditions for hyperbolic transport problems is widespread, and is known to provide increased robustness and more rapid convergence of the numerical solver (see *e.g.* [2, 3]). This is because disturbances that are generated during the iteration are convected out of the domain, instead of reflected from the boundaries until dissipated by numerical viscosity. Careful treatment of artificial boundaries helps to ameliorate the sensitivity of the solution with respect to their placement. Consequently, "windowing" a simulation on a given subregion may be carried out. This is possible because the carrier density, average momentum, and energy are not prescribed independently of each other: as a wave passes through a boundary it is allowed to produce changes in combinations of the components of the state vector which are defined by its projection onto the corresponding left eigenvector.

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References

[1] Gardner, C. L., Jerome, J. W., and Rose, D. J., "Numerical Methods for the Hydrodynamic Device Model: Subsonic Flow", *IEEE Transactions on Computer-Aided Design* 8, 5, 1989, pp. 501-507.

[2] Giles, M. B., "Nonreflecting Boundary Conditions for Euler Equation Calculations, *AIAA Journal*, 28, 12, December, 1990, pp. 2050-2058.

[3] Hedstrom, G. W., "Nonreflecting Boundary Conditions for Nonlinear Hyperbolic Systems", *Journal of Computational Physics*, 30, 1979, pp. 222-237.

[4] Lax, P. D., *Hyperbolic Systems of Conservation Laws and the Mathematical Theory of Shock Waves*, CBMS-NSF Regional Conference Series in Applied Mathematics, Society for Industrial and Applied Mathematics, Philadelphia, PA, 1984.

[5] Lundstrom, M., *Fundamentals of Carrier Transport*, Addison-Wesley, Reading, MA, 1990.

[6] Witham, G. B., *Linear and Nonlinear Waves*, John Wiley and Sons, New York, 1974, pp. 113-142.