Local discontinuous Galerkin methods for moment models in device simulations: formulation and one dimensional results

Yunxian Liu¹ and <u>Chi-Wang Shu</u>

Division of Applied Mathematics, Brown University, Providence, RI 02912 ¹School of Mathematics and System Sciences, Shandong University, Jinan 250100, China

E-mail: shu@dam.brown.edu website: http://www.dam.brown.edu/people/shu We report our preliminary work in applying the local discontinuous Galerkin (LDG) finite element method to solve various time dependent and steady state moment models for semiconductor device simulations, in which both the first derivative convection terms and second derivative diffusion (heat conduction) terms exist and are discretized by the discontinuous Galerkin method and the local discontinuous Galerkin method [3] respectively. The potential equation for the electrical field is also discretized by the local discontinuous Galerkin method. This is an ongoing project with the objective of developing a numerical tool based on the discontinuous Galerkin and local discontinuous Galerkin methodology, capable of solving various models for semiconductor device simulations (hydrodynamic models, energy transport models, quantum drift-diffusion or quantum hydrodynamic models, kinetic models, etc.) in a unified treatment of first and higher spatial derivatives, including those for the potential equations, which would allow easy h-p adaptivity and efficient parallel implementation.

The discontinuous Galerkin method is a finite element method which uses discontinuous piecewise polynomials as basis functions and relies on an adequate choice of numerical fluxes, which handle effectively the interactions across element boundaries, to achieve stable and accurate algorithms for nonlinear hyperbolic conservation laws (those involving first spatial derivatives), nonlinear convection diffusion equations (those involving first, second, and third spatial derivatives), etc., see for example the review paper [3] and references therein. The discontinuous Galerkin method was used before for semiconductor device simulations, such as in [2] for the hydrodynamic models and in [1] for the quantum-hydrodynamic models, however in these carlier works only the convective terms were discretized by the discontinuous Galerkin methodology. Recent development of locally discontinuous Galerkin method in treating higher order spatial derivatives allows us to adopt a unified discretization strategy to handle all spatial derivatives in these models.

In this presentation we describe our preliminary work in one space dimension for simulating the hydrodynamic and energy transport models. In Figure 1 we plot the electron density n and velocity v obtained by the current discontinuous Galerkin algorithm, in comparison with that obtained by the ENO (essentially non-oscillatory) finite difference method, for the hydrodynamic models and the energy transport model, on a one dimensional silicon $n^+ - n - n^+$ diode, see [4] for the details of the HD and ET models, the specifics of the diode, and the ENO finite difference method. We can clearly see that the discontinuous Galerkin algorithm provides very good numerical results in agreement with the results obtained by the ENO finite difference method. While for this one dimensional case the advantage of using discontinuous Galerkin method over the finite difference ENO method is not obvious, the formulation of the discontinuous Galerkin solver does allow an easy generalization to two and higher spatial dimensions on arbitrary triangulations with flexible h-p adaptivity capabilities.

A full journal publication of this work will be published in the Journal of Computational Electronics.



Figure 1: Comparison of the discontinuous Galerkin method (solid lines) with the finite difference ENO method (symbols) for a one dimensional silicon n^+ -n- n^+ diode of length 0.6 μm . Top: hydrodynamic (HD) model; bottom: energy transport (ET) model. Left: electron density n (10¹² cm^{-3}), right: velocity v ($\mu m/ps$).

References

[1] Z. Chen, B. Cockburn, C. Gardner and J. Jerome, *Quantum hydrodynamic simulation of hysteresis in the resonant tunneling diode*, Journal of Computational Physics, v117 (1995), pp.274-280.

[2] Z. Chen, B. Cockburn, J. Jerome and C.-W. Shu, Mixed-RKDG finite element methods for the 2-D hydrodynamic model for semiconductor device simulation, VLSI Design, v3 (1995), pp.145-158.

[3] B. Cockburn and C.-W. Shu, Runge-Kutta Discontinuous Galerkin methods for convectiondominated problems, Journal of Scientific Computing, v16 (2001), pp.173-261.

[4] J. Jerome and C.-W. Shu, Energy models for one-carrier transport in semiconductor devices, in IMA Volumes in Mathematics and Its Applications, v59, W. Coughran, J. Cole, P. Lloyd and J. White, editors, Springer-Verlag, 1994, pp.185-207.

A full journal publication of this work will be published in the Journal of Computational Electronics.