A numerical study of fermi kinetics transport

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Numerical analyses of Fermi kinetics transport illustrate its convergence characteristics. Its adaptation of the Scharfetter-Gummel discretization scheme yields convergence between first and second-order.

Fermi kinetics transport (FKT) uses moments of the Boltzmann transport equation (BTE) to simulate charge transport in semiconductor devices. Its defining feature is electronic heat flow based on the thermodynamic identity and enforcing the second law of thermodynamics [1]. When combined with electronic band-structure and full-wave electromagnetics, it can accurately simulate electronic devices from DC up through mm-wave frequencies without adjustable calibration parameters [2], [3].

This abstract demonstrates FKT's numerical convergence characteristics. Analyses of semiconductor device simulations reveal convergence between first and second-order.

Convergence is quantified by evaluating the relative L^2 error,

$$\in k = \sqrt{\sum_i \; [\widetilde{u}_{i,k} - u_{i,k}]^2 / \sum_i \; u_{i,k}^2} \tag{1}$$

on a series of meshes. Here, $\widetilde{u}_{ik}$ and u_{ik} are numerical and analytic solutions in the i^{th} element of the k^{th} mesh, respectively. First, discrete particle flux divergence is computed with an analytic solution variable profile. The numerical solution is $\widetilde{u}_{ik} == \Sigma_j \, J_{n,ijk,} \, A_{ijk}$, where $J_{n,ijk}$ is the flux through the j^{th} surface with area A_{ijk} of the i^{th} Voronoi polyhedron [3] in the k^{th} mesh. The analytic solution is $u_{ik} = \Sigma_j \, (\nabla . \vec{J}_n)_{ijk} \, \omega_{ijk} V_{ik}$ where ω_{ijk} is the jt^{h} quadrature weight inside the i^{th} Voronoi polyhedron with volume V^{ik} in the k^{th} mesh. Analytic flux divergence is calculated at the j^{th} quadrature point.

Order analyses for electronic device examples are determined in a similar way. The solution $u_{ik} = u_{i,k}^{D} \omega_i V_i$ at the i^{th} quadrature point in the k^{th}mesh is interpolated from the solution set u^D numerically calculated on a dense mesh. The numerical solutions $\widetilde{u}_{ik} = u_{i,k}^{k} \omega_i V_i$ are interpolated from the k^{th} mesh solution set u^k to quadrature points generated in mesh tetrahedra. Errors are calculated with (1).

Figure 1 shows electric potentials and particle fluxes. Flux and flux divergence reconstruction errors in Figure 2 reveal first-order Scharfetter-Gummel discretization. Figures 3 and 5 show GaAs device solution variables with error convergences in Figures 4 and 6 varying between first and secondorder.

FKT is a deterministic BTE solver incorporating the second law of thermodynamics as its closure relation. Several results are presented which provide insights into the discretization techniques. Solving the discretized device equations shows convergence is first-order and higher.

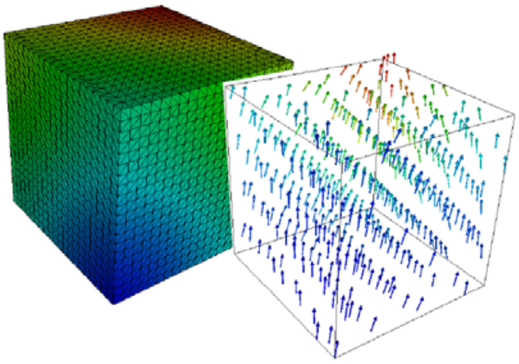

Fig. 1. 3D particle flux reconstruction on the DV mesh. (left) The electric potential profile and (right) the resulting particle flux.

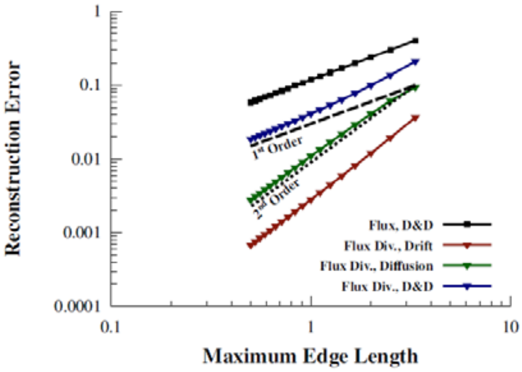

Fig. 2. Error analysis of the FKT flux and flux divergence reconstruction on a series of structured meshes. Here, D&D stands for drift and diffusion. Each mesh reconstruction was compared to an analytic flux and flux divergence as described in Section II.

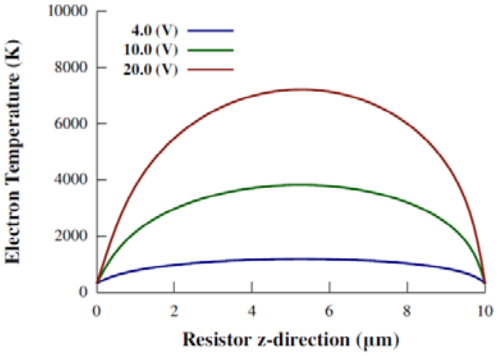

Fig. 3. The electron temperature profiles in the resistor example along the drift axis (the z-axis) for applied biases of 4 V (blue), 10 V (green), and 20 V (red).

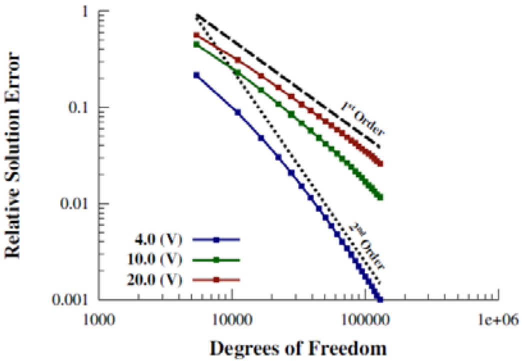

Fig. 4. Error analysis of the fully coupled nonlinear FKT system on a series of structured meshes. The device is a GaAs resistor with applied biases of 4 V (blue), 10 V (green), and 20 V (red). Each mesh solution set was compared to a numerical solution set calculated on a dense mesh.

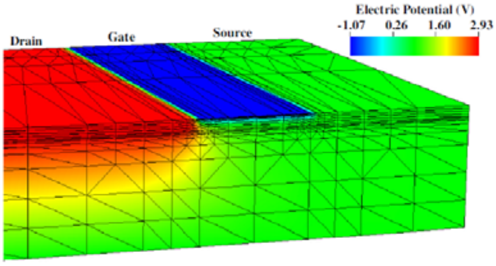

Fig. 5. The electric potential profile in the GaAs MESFET example with a gate bias of -1 V and a drain-source bias of 2 V.

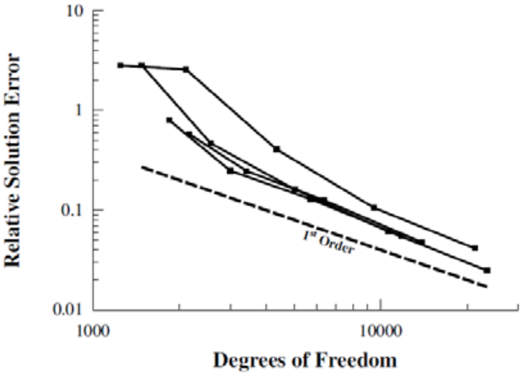

Fig. 6. Error analysis of the fully coupled nonlinear FKT system on a series of device meshes. The device is a GaAs MESFET with an applied gate bias of -1 V and a drain-source bias of 2 V. The multiple error lines correspond to different mesh refinements. Each mesh solution set was compared to a numerical solution set calculated on a dense mesh.

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