A Godunov-type Stabilization Scheme for Solving the Stationary and Transient Boltzmann Transport Equation

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We present a novel deterministic method of solving the coupled system of Poisson's equation and Boltzmann Transport Equation (BTE) using a modified version of the well-established Godunov's scheme [2]. The method is applied to a one-dimensional gallium arsenide (GaAs) Gunn-diode of 1.3 µm length [1], shown in Fig. 1.

The electron's k-space is approximated by 3 isotropic valleys of different multiplicities. Using rotational symmetry along the transport direction allows for projecting the valleys onto a 2D k-space. Triangulation of the k-space along equi-energy spheres yields triangular toroids as finite k-volumes.

Within a spatial cell the potential is approximated piecewise-constant. Therefore, the k-space can be easily discretized via a finite volume method (FVM). Another FVM along the spatial dimension leads to a Riemann problem at the interfaces which is solved by Godunov's scheme under the condition of flux conservation [3].

Numerically stable solutions are obtained under stationary, small-signal as well as transient conditions, see Figs. 1 to 4 and 6. The positivity of the electron's phase space distribution is fulfilled by construction even when considering GaAs's polar optical phonon which shows highly angle-dependent scattering behavior. Godunov's scheme introduces strong artificial damping at frequencies above 10 THz, but refining the spatial grid leads to a reduction in damping, cf. Fig. 5.

Godunov's scheme yields a straight-forward approach to implement transient simulations which is stable even for the Forward Euler scheme but implicit schemes are more efficient. First order implicit time integration methods, e.g. the Backward Euler (BE) method, introduce another source of artificial damping. By using higher-order methods, such as a trapezoidal rule (TR) or BDF2, one can reduce the damping as can be seen in Fig. 6 where a constant time step has been chosen for better comparison. Since we applied an ideal voltage source Gunn-oscillations are suppressed.

Oscillations can occur when the admittance has a negative real part (see Fig. 4) and a finite load is attached. The largest negative real part of the admittance at 3V DC is found at 150 GHz near which the most powerful oscillations might occur.

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References

[1] S. García et al. "Time-domain Monte Carlo simulations of resonant-circuit operation of GaN Gunn diodes". In: *2013 Spanish Conference on Electron Devices*. 2013, pp. 79–82. DOI: 10.1109/CDE.2013.6481347.

[2] S. K. Godunov. "A difference method for numerical calculation of discontinuous solutions of the equations of hydrodynamics". In: *Matematicheskii Sbornik* 47(89) (3 1959), pp. 271–306.

[3] Maziar Noei, Tobias Linn, and Christoph Jungemann. "A numerical approach to quasi-ballistic transport and plasma oscillations in junctionless nanowire transistors". In: *Journal of Computational Electronics* 19 (2020), pp. 975–986. DOI: 10.1007/s10825-020-01488-4.

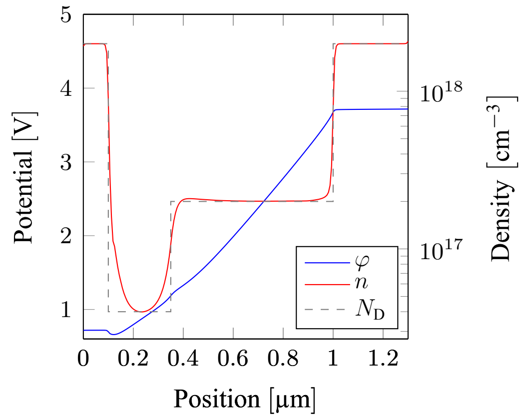

Figure 1: Potential φ, electron density n, and donator doping N_{D}.

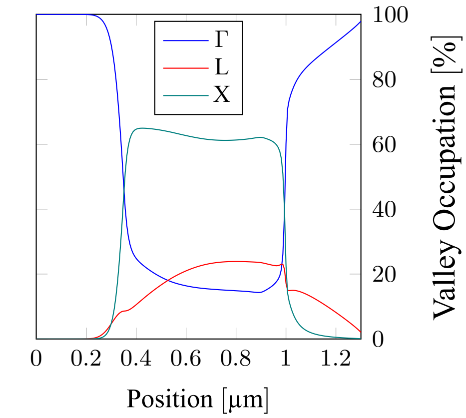

Figure 2: Valley occupation numbers o^{ν} for $\nu = \Gamma, \mathrm{L}, \mathrm{X}$ valleys.

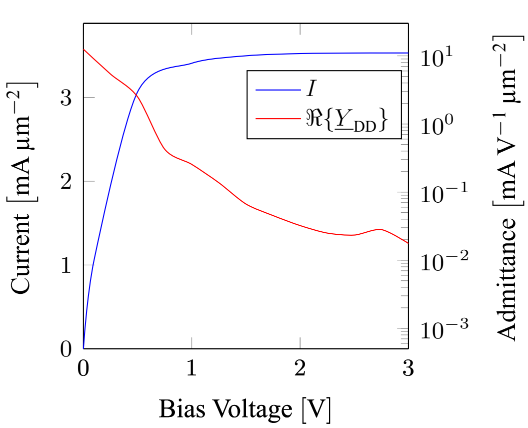

Figure 3: Current-voltage characteristic and real part of admittance $\Re\{\underline{Y}_{\mathrm{DD}}\}$ at $f = 0\,\mathrm{Hz}$.

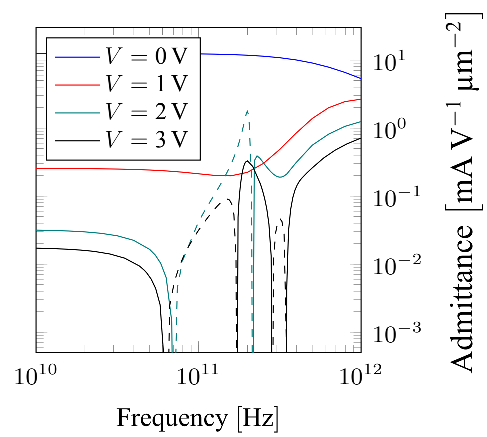

Figure 4: Real part of admittance $\Re\{\underline{Y}_{\mathrm{DD}}\}$ for multiple bias points V. Dashed lines indicate intervals of negative real part.

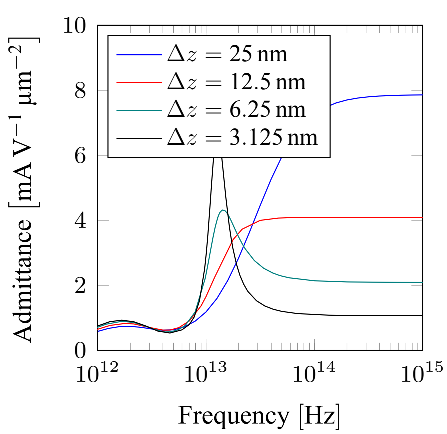

Figure 5: Real part of admittance $\Re\{\underline{Y}_{\mathrm{DD}}\}$ at high frequencies f for multiple spatial grid spacings Δz.

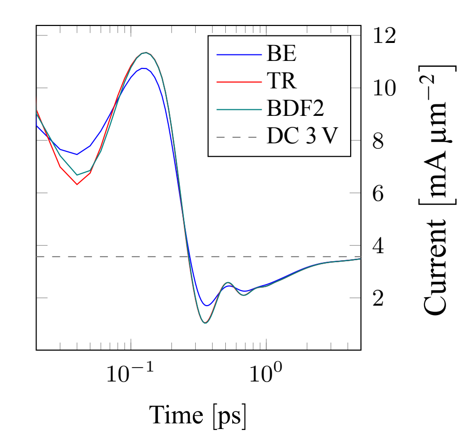

Figure 6: Current evolution for an instantaneous change in bias voltage from 0 to 3 V. All time integration schemes use a constant time step of $\Delta t = 10\,\mathrm{fs}$.

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