

# HARMONIC SOLUTION OF SEMICONDUCTOR TRANSPORT EQUATIONS FOR MICROWAVE AND MILLIMETRE-WAVE DEVICE MODELLING

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**Abstract** - The transport equations for charges in a semiconductor have been solved for a periodic voltage excitation by means of a harmonic approach, for modelling of microwave and millimetre-wave active devices. The solution is based on the expansion of the unknown physical quantities in Fourier series in the time domain, and on the discretisation in the space domain. A Waveform-Balance technique in the time domain is used to solve the resulting non-linear equations system. In this way the time step is determined only by Nyquist's sampling requirements at the operating frequency, irrespective of the relaxation times of the semiconductor. This approach allows for a longer time step, and therefore a shorter computing time, than a space- and time-discretised standard solution for many cases of interest, opening the way to effective device simulation.

## I. THE TRANSPORT EQUATIONS

The efficient solution of the equations describing the behaviour of charges in the active region of a device is the basis for an effective physical modelling for CAD applications. A suitable set of transport equations are the first three moments of Boltzmann's transport equation [1], i.e. particle conservation (continuity), particle momentum conservation and particle energy conservation, together with Poisson's equation. The system is a non-linear partial differential equation system with respect to time and space, that for simplicity is here reported for only one dimension in space:

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{q(N_d - n)}{\epsilon}$$

$$\frac{\partial n}{\partial t} = -\frac{\partial(nv)}{\partial x}$$

$$\frac{\partial v}{\partial t} = -\frac{v}{m_{eff}} \frac{\partial(m_{eff} v)}{\partial x} + \frac{qE}{m_{eff}} - \frac{2}{3nm_{eff}} \frac{\partial}{\partial x} \left( nv - \frac{1}{2} m_{eff} nv^2 \right) - \frac{v}{\tau_v}$$

$$\frac{\partial w}{\partial t} = -v \cdot \frac{\partial w}{\partial x} + qvE - \frac{2}{3n} \cdot \frac{\partial}{\partial x} \left( nvw - \frac{1}{2} m_{eff} nv^2 \right) - \frac{(w - w_0)}{\tau_w}$$

The applied voltage is the forcing term, and appears as the boundary condition of Poisson's equation. In the traditional approach [2] the equations are discretised with respect to both time and space, and the resulting finite-difference system is solved numerically:

$$\frac{\psi_k^{j+1} - 2\psi_k^j + \psi_k^{j-1}}{(\Delta x)^2} = \frac{q}{\epsilon} (n_k^j - N_d)$$

$$\frac{n_k^j - n_{k-1}^j}{\Delta t} = -n_k^j \frac{(v_k^{j+1} - v_k^{j-1})}{\Delta x} - v_k^j \frac{(n_k^{j+1} - n_k^{j-1})}{\Delta x}$$

$$\frac{v_k^j - v_{k-1}^j}{\Delta t} = -\frac{v_k^j}{m_{eff,k}^j} \left[ \frac{m_{eff,k}^{j+1} v_k^{j+1} - m_{eff,k}^{j-1} v_k^{j-1}}{2\Delta x} \right] + \frac{qE_k^j}{m_{eff,k}^j} + \frac{qE_{a,k}^j}{m_{eff,k}^j v_k^j}$$

$$\frac{w_k^j - w_{k-1}^j}{\Delta t} = -v_k^j \cdot \frac{w_k^{j+1} - w_k^{j-1}}{2\Delta x} + q(E_{ss,k}^j v_{ss,k}^j - E_k^j v_k^j)$$

where the subscript  $k = 0, \dots, K$  refers to the time instant and the superscript  $j = 0, \dots, J$  refers to the position in space in the one-dimensional sample. The diffusion terms have been neglected for simplicity. Starting from an initial value  $n_0$  at  $t = t_0$  for all positions in the sample the system is solved time instant after time instant, for all positions in space at the same time; since it is non-linear, an iterative Newton-Raphson algorithm is used. This requires the inversion of a Jacobian matrix of order  $J$  (the number of space steps in the sample), that is 3-diagonal for each equation.

In order for the algorithm to converge the discretisation steps must be smaller than a minimum quantity. In particular, the step of the time variable must be smaller than the energy, momentum and dielectric relaxation times. This



is a major problem when a solution in the microwave or millimetre-wave frequency range is required, because the required time step is in the range of  $\Delta t \cong 10^{-14} \div 10^{-15}$  s, while the analysis must be performed for a minimum time interval equal to the microwave or millimetre-wave period, i.e.  $T = 10^{-9} \div 10^{-11}$  s, or a number of time steps in the order of  $n_T = 10^3 \div 10^6$ . The number of time steps is extremely large, and the computing time very high.

## II. THE HARMONIC APPROACH

In the time- and space-discretised approach the number of time steps is in fact unnecessarily large, because the very fine resolution in time is not required for the signal analysis, as it corresponds to frequency components much higher than the microwave or millimetre-wave frequency band; it is nonetheless required for the convergence of the discretised system. A different approach has been adopted in our case.

The equations are first discretised in space, so that the right-hand-side of the system becomes the same as in the time- and space-discretised case; the left-hand-side so far remains as in the original equations. Given the periodicity in time of the applied excitation, all the quantities (i.e. potential, electron density, velocity and energy) and their time derivatives at each position  $j$  are expanded in Fourier series in time, with fundamental frequency as that of the applied signal (we report the expressions for the electron density only):

$$n^j(t) = \sum_p N_p^j \cdot e^{ip\omega t}$$

$$\frac{\partial n^j(t)}{\partial t} = \sum_p jp\omega \cdot N_p^j \cdot e^{ip\omega t}$$

$$p = -P, \dots, P \quad j = 0, \dots, J$$

where the subscript  $p$  refers to the harmonic of the signal frequency. The phasors  $N_p^j$  are computed from  $(2P+1)$  samples of  $n(t)$  in the period  $T = 2\pi/\omega$  (Nyquist's sampling theorem):

$$n^j(t_k) = \sum_p N_p^j \cdot e^{ip\omega t_k}$$

$$N_p^j = \frac{1}{2\pi} \sum_k n(t_k) \cdot e^{-jp\omega t_k}$$

$$t_k = \frac{k}{2P+1} \cdot T \quad k = -P, \dots, P$$

The number of samples  $(2P+1)$  in a period  $T$  (and therefore the correspondent time step) is set with reference only to

the maximum frequency of interest, i.e. the  $P$ -th harmonic of the signal. By using the expression for phasors the time derivatives can be expressed as:

$$\frac{\partial n^j(t_k)}{\partial t} = \sum_k c_k \cdot n^j(t_k) = \sum_k c_k \cdot n_k^j$$

i.e. the time derivative at the time instant  $t_k$  at the position  $j$  is expressed as a function of the values at the same position  $j$  at all sampling time instants. The values of the coefficients  $c_k$  are plotted in fig. 1 in the case of  $P=5$ .

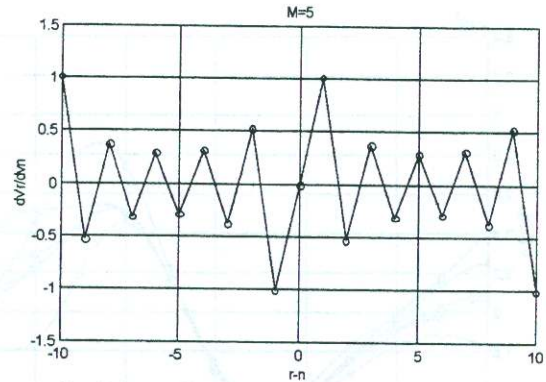


Fig. 1 The coefficients of the time derivative for  $P = 5$

Replacing the expression for the derivative in the left-hand-side, the equations now cannot be solved time instant after time instant as in the case of the traditional time- and space discretisation, since all time samples  $n(t_k) = n_k$  are present in the left hand side of the equations at each time instant  $t_k$ . A consequence is that the Jacobian matrix of the global system (for all time instants and positions in space) is now  $(4P+3)$ -diagonal (23 in the case of  $P = 5$ , i.e. 5 harmonics) for each equation; however the system is solved only once for the whole period, while the traditional time-discretised approach requires the solution of a 3-diagonal matrix for each time instant, that usually means a very great number of points, as already remarked.

This is a consequence of the harmonic approach, where the general form of the time dependence is a priori fixed as a superposition of harmonic sinusoids, whose coefficients depend on the global behaviour of the variable in the whole period. In this 'integral' approach the value of the derivative somehow 'averages' the behaviour within a period, filtering out the too-high frequency components due to too-small time constants, and limiting the number of time samples to the minimum value.

## III. IMPLEMENTATION AND RESULTS

Both algorithm have been implemented for a one-dimensional semiconductor sample. In this first validation phase some terms have been neglected in the equations for



the sake of simplicity, while retaining the generality of the approach. Poisson's and continuity equations are solved simultaneously because of their strong coupling; the other two conservation equations are solved iteratively, recomputing the values of the relaxation time constants, until the solution converges to a stable value [3]. In fig. 2 the electron velocity in a section of the sample is plotted vs time (one period) for several iteration steps: it is apparent the convergence toward the solution. Similarly, in fig. 3 the velocity is plotted for a time instant vs space (the length of the sample) for several iteration steps. The simultaneous convergence in both time and space is clearly shown.

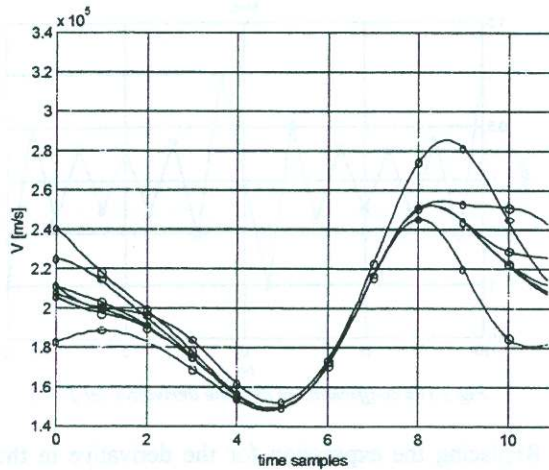


Fig.2 – Velocity of a particle in a section of the semiconductor sample ( $x=0.8 \mu\text{m}$ ) vs time (one period). The solution is shown as it approaches convergence. The sampling instants are indicated.

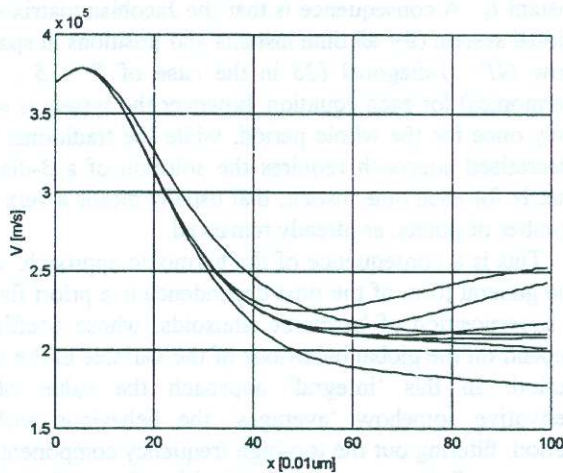


Fig.3 – Velocity of a particle for a time instant in the period ( $t=0$ ) vs space (the semiconductor sample). The solution is shown as it approaches convergence.

In fig.4 the spectra (amplitude, dB, and phase, radians) of the velocity as a function of time and space are shown for fundamental frequency and 4 harmonics (plus DC).

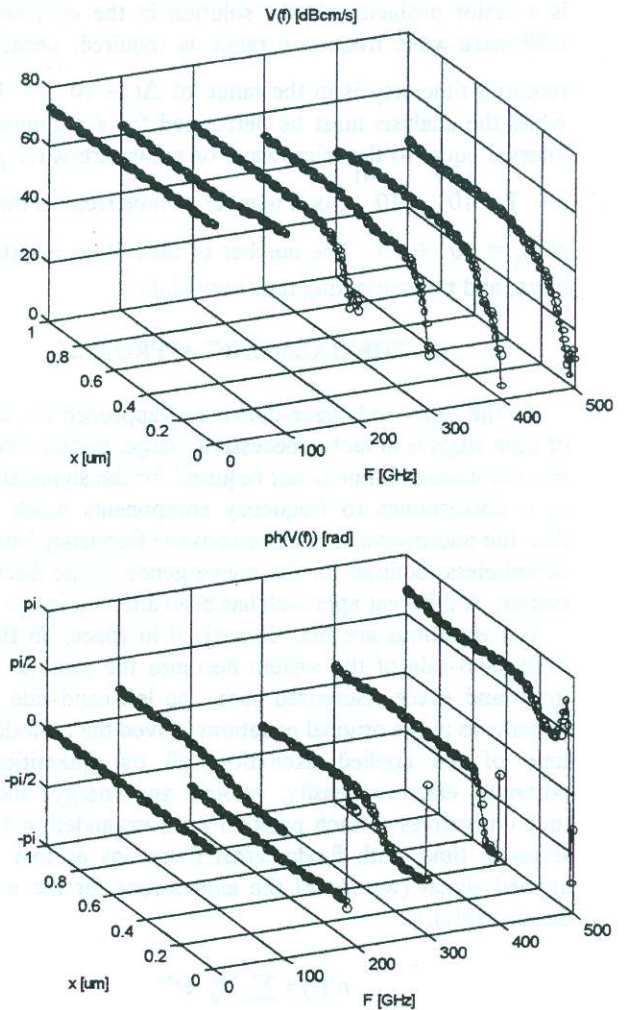
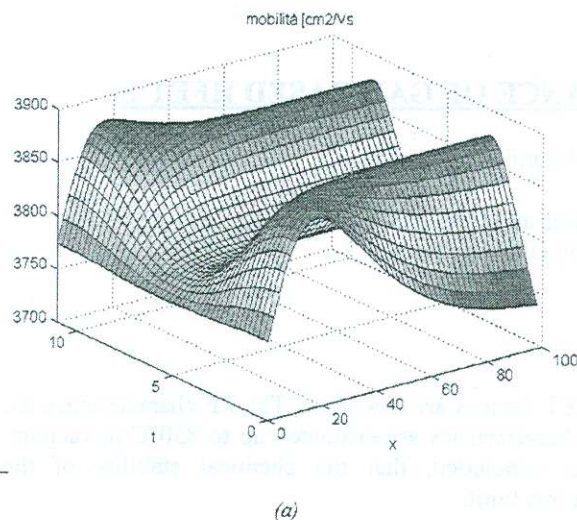


Fig.4 – Spectra of the velocity (amplitude, dB, and phase, radians) as a function of time and space in the semiconductor sample

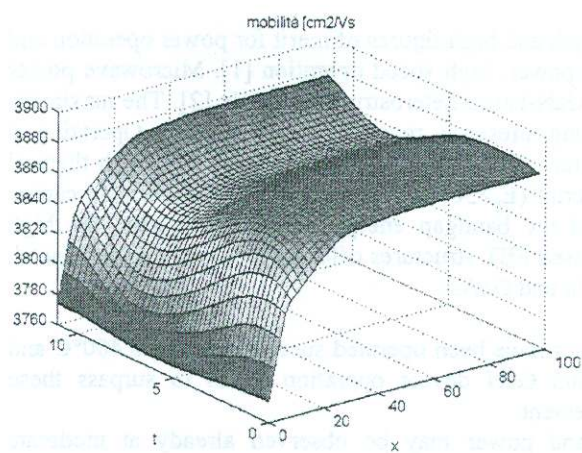
Many cases have been analysed using the proposed harmonic approach, and they have been compared to the traditional, time- and space-discretised solution, for a one-dimensional semiconductor sample at several operating frequencies from the low microwave to the sub-millimetre-wave ranges. The results are practically identical for the two methods, as expected, but the computing times are very different.

In fig. 5 the electron mobility is shown as a function of time and space for a GaAs sample  $1 \mu\text{m}$  long, with doping density  $N_D = 10^{23} \text{ m}^{-3}$ , and an applied sinusoidal voltage of amplitude  $V_s = 0.15 \text{ V}$  around a bias voltage  $V_{DC} = 0.3 \text{ V}$  at a frequency of  $5 \text{ GHz}$  and  $500 \text{ GHz}$ , computed with the time-harmonic method. For the lower frequency the velocity overshoot at the beginning of the sample is clearly shown for the part of the period when the field is high. For very high frequency the electrons cannot follow the applied signal because of the relaxation times of the semiconductor.





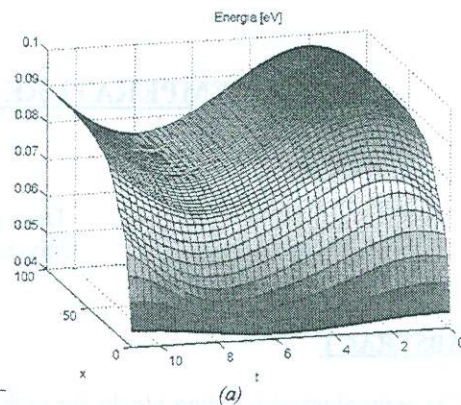
(a)



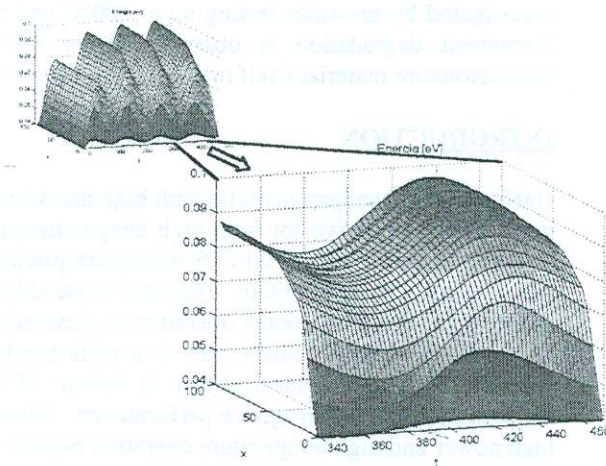
(b)

Fig.5 Electron mobility as a function of time and space for a frequency of 5 GHz (a) and 500 GHz (b)

In fig. 6 the electron energy is plotted at 500 GHz as computed with the proposed harmonic approach (a) and with the traditional time- and space-discretised method (b). The comparison shows that the results are practically identical; with the time-discretised method more than one period must be analysed at very high frequency in order to reach the steady-state periodic regime. The time-harmonic solution, computed for 5 harmonics, requires a computing time of 3.4 s in all cases, while the traditional time- and space-discretised solution requires 3285, 550 and 443 s at 5, 50 and 500 GHz respectively. The robustness of the algorithm also proves to be greater in the time-harmonic case. The code is written in C language for a PC.



(a)



(b)

Fig.6 – Electron energy as a function of time and space for a frequency of 500 GHz with the harmonic approach (a) and the time- and space-discretised method (b) with steady-state regime expanded for comparison.

In conclusion, a new harmonic approach to the solution of the transport equation together with Poisson's equation in a semiconductor proves to be faster, more flexible and robust than the traditional approach, opening the way to the effective simulation of active devices for microwave and millimetre-wave circuit applications.

#### IV. REFERENCES

- [1] K. Bløtekjær, "Transport Equations for Electrons in Two-Valley Semiconductors," *IEEE Trans. on Electron Devices*, vol. ED-17, pp. 38-47, Jan. 1970.
- [2] S. Selberherr, *Analysis and Simulation of Semiconductor Devices*, Springer-Verlag/Wien, New York 1984.
- [3] T. Shawki, G. Salmer, O. El Sayed, 'MODFET 2-D hydrodynamic energy modelling: optimisation of subquarter-micron-gate structures', *IEEE Trans. Electron Devices*, vol.37, pp.21-29, Jan. 1990.