Elimination of numerical underflow in the modelling of optoelectronic devices using multiple precision

S.N. Kaunga-Nyirenda, J.J. Lim[1], S. Bull and E.C. Larkins[1]
[1]The University of Nottingham, University Park, Nottingham, NG7 2RD, U.K.

Abstract – **In 2D and quasi-3D simulations, Fermi-level pinning of the surfaces has been found to result in the decoupling of the electron and hole populations, preventing numerical convergence to the correct solution. In this work, we report on the elimination of numerical underflow in the self-consistent solution of the Poisson and continuity equations in a 2D optoelectronic device simulator. The use of extended precision to represent the state variables eliminates the numerical underflow and consequently the decoupling of the electron and hole populations.**

I. Introduction

Photonic integration is becoming an increasingly important area of research to satisfy the growing demand for ultra-high bandwidth applications. Photonic crystal (PhC) technology is a promising candidate for such applications, due to its ultra-low power consumption and extreme compactness. Numerical modelling continues to play an important role in the design and development of novel device structures and technologies. Compact receivers and switching components are key devices in achieving optoelectronic integration. PhC All-optical gates (AOGs) and photodetectors are central building blocks for these components. Understanding their operation is therefore of utmost importance.

Carrier transport plays an important role in device operation. Due to their 3D structure, small dimensions and large surface to volume ratio, 2D and 3D spatial models are needed for modelling PhC AOGs and phototedetectors. In most analyses, numerical simulation of carrier transport has been based on self-consistently solving the basic semiconductor equations consistently and equations for the optical fields. However, it has been observed that the solutions of Poisson and continuity equations in 2D and 3D simulations of PhC AOGs and photodetectors do not always converge. This problem is particularly prevalent when Fermi-level pinning in included in the 2D and 3D simulations. This lack of convergence arises from numerical underflow in the addition of the majority and minority carrier charge for the solution of Poisson's equation, which results in the numerical decoupling of the electron and hole populations. This problem also affects the simulation of conventional optolectronic devices, where the separation between the Fermi level and the band edges is large. This includes photodetectors, laser diodes at low bias, wide bandgap devices and multiple junction devices e.g. p-n-p-n diodes.

II. Solution to numerical underlow problem

The problem described above arises from the treatment of values that vary over a large range in the Newton algorithm and therefore prevent convergence. Standard double precision only has approximately 16 decimal digits, which leads to numerical underflow in Poisson's equation and the decoupling of the electron and hole populations. Different approaches have been employed to deal with the problem of convergence in the Newton solver. One approach is to keep densities above a certain minimum value at all stages of the simulation [1]. This is artificial, as it fails to track the actual values and may alter the contribution of certain processes to the overall device behavior. Another method common in device simulation is the use of linear sparse solvers with iterative refinement [2]. In this case, the corrections are still solved for in double precision, while the update step is done in higher precision. This has been found to improve the stability of the solution. However, this is not satisfying, since the source of the problem is the variation in the different contributions to the Poisson and continuity equations and this approach does not actually remove the problem of numerical underflow. The most robust solution requires that the state variables themselves be represented in higher precision. This requires that the linear sparse solver itself should be implemented in higher precision, rather than just the updates as is the case with iterative refinement.

III. Extended Semiconductor device simulator

The details of our in-house electro-opto-thermal semiconductor device simulator have been presented elsewhere [1], [4]. It is a well established 2D/quasi-3D simulation tool, which self-consistently solves the Poisson and continuity equations, coupled to equations describing the optical fields (e.g. photon rate equations, finite difference beam propagation method). The present work extends the simulator to multiple precision to eliminate the problem of numerical underflow encountered when surface effects are introduced in 2D simulations. An existing linear sparse solver has been extended to multiple precision. All the important state variables are stored in multiple precision. The 2D electrical solver includes the surface Fermi level pinning based on Spicer's unified defect theory [5], [6], following the numerical approach described by Darling [7].

IV. Results and Discussions

Full 2D electrical simulations were performed using the extended simulator with quadruple precision at equilibrium. Under equilibrium conditions, the quasi-Fermi levels should converge to flat Fermi level, which is continuous throughout the device. Fig 1 shows the band structure obtained using double precision at equilibrium. Clearly, the quasi-Fermi levels do not converge to the flat Fermi level, as required for equilibrium. This clearly demonstrates the decoupling of the electron and hole populations, which results from numerical underflow in Poisson's equation. Fig. 2 shows the results of the same simulation of the same structure obtained using the simulator with extended precision. The quasi-Fermi levels merge with the equilibrium Fermi level and the problem of

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numerical underflow disappears. The performance of this extended model is now being benchmarked for the simulation of other photonic devices, including laser diodes and photodetectors. Initial indications suggest, however, that the penalty in terms of computation time is modest (i.e. less than a two-fold increase when moving from double precision to quad precision).

V CONCLUSIONS

We have presented an extended semiconductor device simulator based on multiple precision, which deals with the problem of numerical underflow in Poisson's equation and continuity equations when surface effects are taken into account in 2D. This extends the capability of our 2D and quasi-3D semiconductor device simulators, allowing them to accurately deal with the physics of the surface, including surface charging and surface Fermi-level pinning and their effect on the operation of optoelectronic devices. As devices get smaller in dimensions, surface effects become increasingly important and their correct treatment is of importance. Benchmaking in terms of overheads on the simulation requirements is currently being performed, but initial results suggest only a modest computational penalty. Treatment of other devices where similar problems are encountered will be of great interest and importance to the semiconductor device design.

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REFERENCES

[1] S. Steiger, R.G. Veprek and B. Witzigmann, "Unified simulation of transport and luminescence in optoelectronic nanostructures", *J. Comput Electron*, Vol 7, pp. 509-520, 2008

[2] T. Tayabe, H. Masuda, Y. Aoki, H. Shukuri and T. Hagiwara, "Three-dimensional device simulator CADDETH with highly convergent matrix solution", *IEEE Trans. Elect. Device.,* Vol ED-32, No 10, pp 2038-2044

[3] J.J. Lim, R. MacKenzie, S. Sujecki, E.C. Larkins, M. Sadeghi, S.M. Wang, Y.Q. Wei, J.S. Gustavsson, A. Larsson, P. Melanen, P. Sipilä, P. Uusimaa, A.A. George and P.M. Smowton, "Simulation of DQW GaInNAs Laser Diodes," *IET Optoelectronics*, Vol. 1, No. 6, pp. 259-265, 2007.

[4] J.J. Lim, R. MacKenzie, S. Sujecki, M. Sadeghi, S.M. Wang, G. Adolfsson, Y.Q. Wei, A. Larsson, P. Melanen, P. Uusimaa, A.A. George, P.M. Smowton and E.C. Larkins, "Thermal performance investigation of DQW GaInNAs laser diodes," submitted to *Opt. Quantum Electron.*, NUSOD special issue, 2007.

[5] W.E. Spicer, T. Kendelewicz, N. Newman, R. Cao, C. McCants, K. Miyano, I. Lindau, Z. Liliental-Weber, and E.R. Weber. "The advanced unified defect model and its applications." Applications of Surface Science Vol. 33/34, pp. 1009-29, 1988.

[6] W. E. Spicer, Z. Liliental-Weber, E. Weber, N. Newman, T. Kendelewicz, R. Cao, C McCants, P. Mahowald, K. Miyano and I. Lindau. "The advanced unified defect model for Schottky barrier formation." Journal of Vacuum Science & Technology B, Vol. 6, No. 4, pp. 1245-51, 1988.

[7] R.B. Darling "Defect-state occupation, Fermi-level pinning, and Illumination effects on free semiconductor surfaces." Physical Review B Vol. 43, No. 5, pp. 4071-83, 1991.

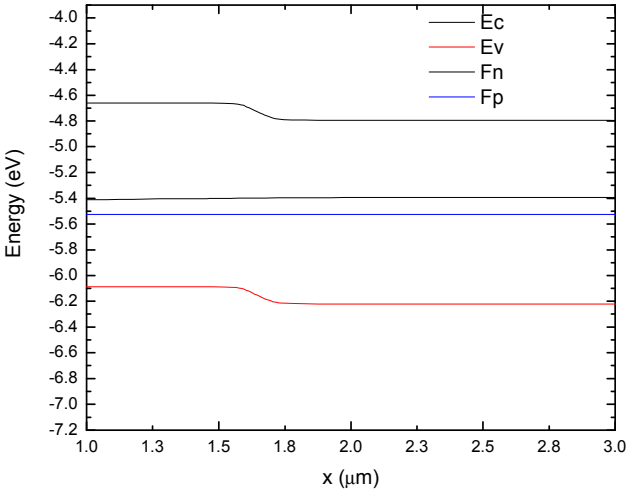

Fig. 1. Band structure of pn junction at equilibrium using the double precision simulator

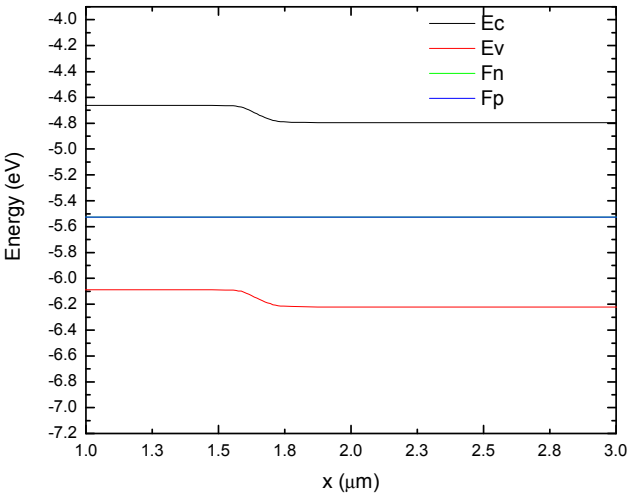

Fig. 2. Band structure of pn junction at equilibrium using the multiple precision simulator