Numerical Aspects of the Deterministic Solution of the Wigner Equation

Johann Cervenka and Lado Filipovic

Institute for Microelectronics, TU Wien, Austria
Johann.Cervenka@TUWien.ac.at

Quantum mechanical effects in the carrier transport processes have to be accounted for during the development of modern and future electronic devices. A convenient formulation is provided by the Wigner formalism [1,2]. Especially for problems where phase-space quantities vary over several orders of magnitudes deterministic solution methods [3] are favored over stochastic approaches. The problematic discretization of the diffusion term triggered the development of an approach which utilizes an integral formulation of the Wigner equation [4]. In general, the developed method describes the evolution in time as the superposition of the time evolution of several fundamental wave packages.
Major considerations are necessary to overcome the memory and time demands typical for the modeling of any quantum transport method [5].
Through an examination of the resulting equations it was possible to dramatically reduce the complexity of the equation system and a final reduced set of equations resulted. However, due to the computational costs of the solving mechanism a parallelization of the procedure is essential and through this approach made possible. Depending on the problem type several solution approaches are feasible which affect the discretization and offer further possibilities for optimization.
Several aspects of the numerical consequences of this approach will be discussed.
For simple problems with a time invariant setup each fundamental evolution can be computed independently, collecting all fundamental solutions to the entire one. Parallelization among the partial processes is made possible.
If a dependence of the partial evolutions is caused, for instance by scattering, the partial processes may be calculated in parallel but the synchronization of and the communication between the processes is required.
If the applied potential stays constant, the partial updates stay constant as well. In this case the partial updates may be calculated only once and applied to the distributions of the previous time-step. However, In this case a communication of the actual solution among the processes has to be triggered.
Depending on the chosen method different computational issues may arise. To achieve the results in reasonable time attention has to be kept on the (at least) second order dependence of spatial and k-space resolution on calculation times. Due to the high dynamic of the solution it may be also necessary to apply a dense time-spacing. Accordingly, in areas of low velocities, due to numerical reasons, the discrete trajectories may stop evolving.
This aspect may not be harmful using stochastic methods. These areas move their discrete position with low probability. In the deterministic version this instance is accounted for by adapting the velocities by their cumulative error in the trajectory in time.
However, for the one-step method, the trajectory update is only calculated once. In this case an interpolation of the solution achieves a result. Attention has to be paid to the fact that information is lost and edges may broaden during this interpolation. In Fig. 1 sample simulations by applying the developed method are shown for a wave packet passing through a 0.1eV potential barrier and through two 0.05V potential barriers.

1. Griffiths, D.: Introduction to Quantum Mechanics. Pearson Prentice Hall, Upper Saddle River (2005)
2. Kosik, R.: Numerical challenges on the road to NanoTCAD. Ph.D. thesis, Institute for Microelectronics (2004)
3. Fu, Y., Willander, M.: Electron wave-packet transport through nanoscale semiconductor device in time domain. J. Appl. Phys. **97** (9), 094311 (2005)
4. Nedjalkov, M., et al.: Unified Particle approach to Wigner-Boltzmann transport in small semiconductor devices. Phys. Rev. B **70**, 115319 (2004)
5. Sellier, J.M.D., et al.: A benchmark study of the Wigner Monte Carlo method. Monte Carlo Method Appl. **20** (1), 43–51 (2014)

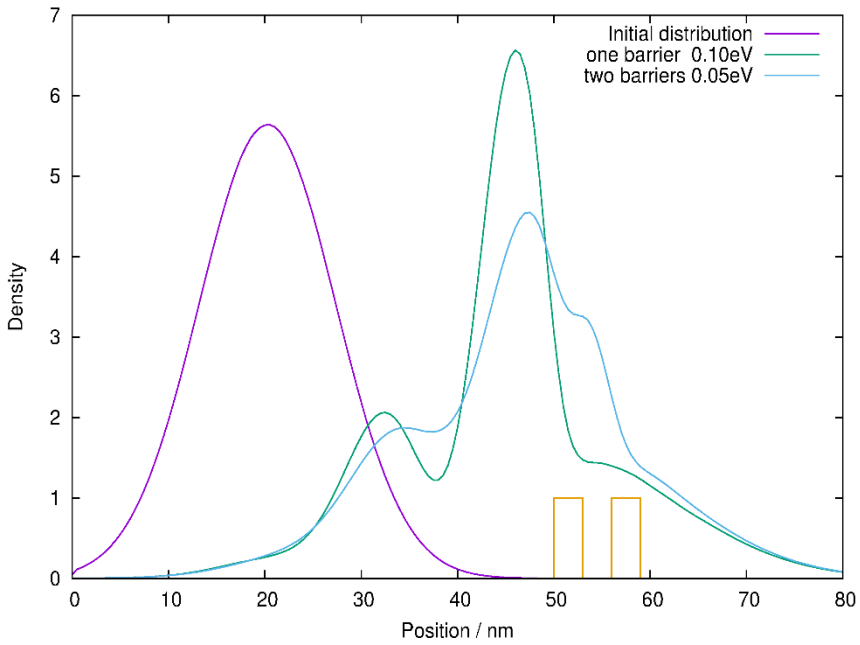

Fig. 1: Two simulations of a wave packet passing through a 0.1eV potential barrier and two 0.05eV barriers are shown at time=0s and after 100fs. In this case the one-step algorithm, in combination with interpolation, achieves best results.