Special Session on

# Advanced Numerical Techniques for PDEs and Applications

## Deterministic Solution of the Discrete Wigner Equation

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To describe the carrier transport processes in novel nanoelectronic devices the effects of quantum mechanics have to be considered as well. The Wigner formulation of quantum mechanics provides a convenient phase space formulation of quantum theory. In this formulation deterministic methods show difficulties in the discretization of the diffusion term in the differential equation. Indeed even high-order schemes show very different output characteristics because of rapid variations of the Wigner function in the phase-space. The developed approach uses an integral formulation of the Wigner equation so that the differentiation can be avoided. We consider the evolution of an initial condition described by the superposition (in phase-space) of particular fundamental wave packages. To calculate the distribution at desired time-steps, the Wigner equation has to be solved for each packet and all ”fundamental evolutions” of have to be summated.
Unfortunately, the usual approach to solve sequentially for each time-step is not practicable due to the huge memory consumption. In the usual case, during time evolution the complete history in phase-space of each point has to be stored. To overcome this drawback, the calculation order is modified in such a way that for each point its specific time evolution is calculated which has to be stored.
As the particular calculations are independent from each other, this method is well suited for parallelization using MPI and OpenMP.
The deterministic results are compared with results obtained from a stochastic approach as well as with solutions of the Schroedinger equation.