Comparison of Slab and Block Decomposition Strategies for the Two-Dimensional Wigner Monte Carlo Method

Josef Weinbub, Paul Ellinghaus, Mihail Nedjalkov, and Siegfried Selberherr
Institute for Microelectronics, TU Wien, Gußhausstraße 27-29/E360, 1040 Vienna, Austria
e-mail: weinbub@iue.tuwien.ac.at

Both stochastic and deterministic methods have been applied to solve the one-dimensional Wigner equation. However, only the Wigner Monte Carlo method, using the signed-particle technique [1], has made multi-dimensional Wigner simulations viable thus far [2]; a multi-dimensional approach is essential for the simulation of realistic semiconductor devices. The primary challenge lies in the fact that the essential *annihilation* algorithm requires the entire phase space to be represented by an array whose size is proportional to the dimensionality and resolution of the phase space – this quickly results in exorbitant memory requirements which easily exceed the limited memory of a single workstation [3]. A spatial domain decomposition approach has been introduced for the one-dimensional Wigner Monte Carlo method [3] and successfully extended to two-dimensional simulations [4]. The implementations use a message passing interface (MPI) technique and are based on the Wigner Ensemble Monte Carlo simulator which is part of the free open source ViennaWD simulation package [5].

Two domain decomposition techniques – a uniform slab and a uniform block decomposition – for two-dimensional problems are compared. The performance of the two approaches is evaluated by simulating a representative physical problem. Figure 1 shows the evolution of three wave packets over 300fs within a 128nm x 128nm simulation, providing 16 dopants acting as potential barriers. Our results (Figure 2) for 16, 32, 64, and 128 MPI processes show that the slab decomposition method is superior to the block decomposition approach. This result is especially interesting, as it shows that the much simpler to implement slab decomposition method is an excellent method for parallelizing highly memory intensive two-dimensional Wigner Monte Carlo quantum simulations based on the signed-particle method.

The computational results have been achieved using the Vienna Scientific Cluster (VSC).

[1] M. Nedjalkov et al., Phys. Rev. B, **70**(11), DOI:10.1103/PhysRevB.70.115319 (2004).
[2] J. Sellier et al., Comput. Phys. Commun., **185**(10), DOI:10.1016/j.cpc.2014.05.013 (2014).
[3] P. Ellinghaus et al., J. Comput. Electron., **14**(1), DOI:10.1007/s10825-014-0635-3 (2015).
[4] J. Weinbub et al., J. Comput. Electron., DOI:10.1007/s10825-015-0730-0 (2015).
[5] ViennaWD, http://viennawd.sourceforge.net/.

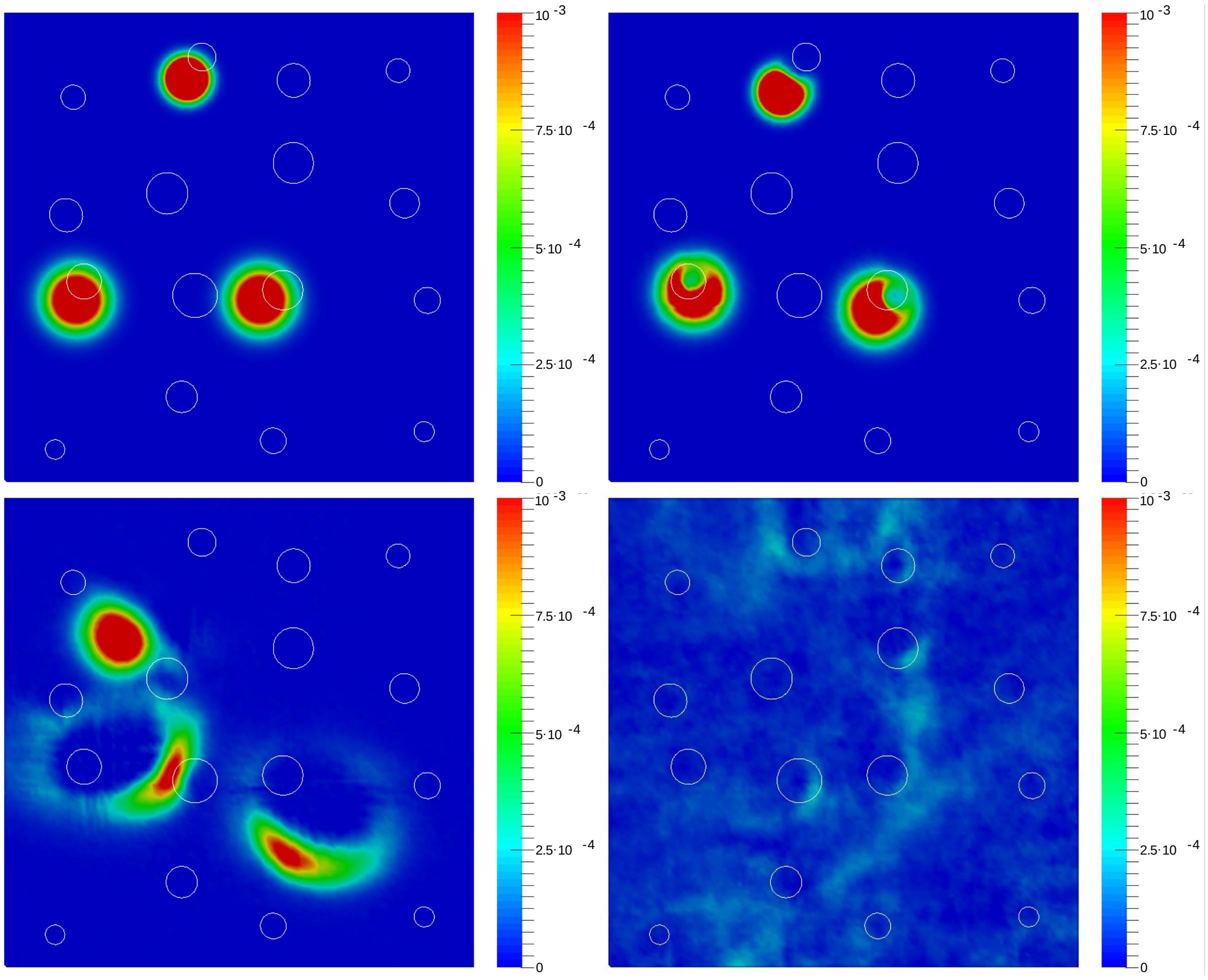

Figure 1: Normalized density (i.e. probability) at 0 fs, 10 fs, 50 fs, and 300 fs (top left, top right, bottom left, bottom right). White cricles denote locations of dopants.

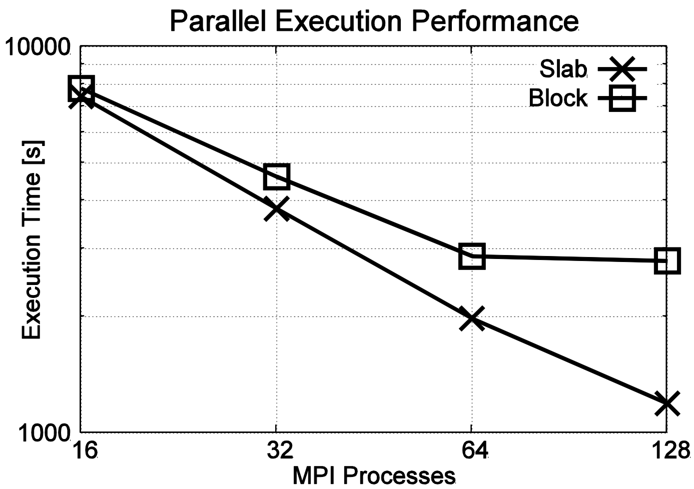

Figure 2: Comparison of the execution times between the slab and the block decomposition approaches.