# Improved Particle Annihilation for Wigner Monte Carlo Simulations on a High-Resolution Mesh

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The effects of surface roughness on quantum transport in modern transistor architectures, e.g. UTB-SOI, have become significant [1]. However, to properly model the surface roughness of a $Si/SiO_2$ interface requires a fine spatial resolution. We investigate the implications of the latter on the Signed-Particle Wigner Monte Carlo (SPWMC) method, which presents a convenient formalism to investigate transient and stationary processes in multi-dimensional semiconductor structures, ranging from quantum-coherent to scattering-dominated transport. Fig. 1 shows how the effective channel width, and thereby the current (Fig. 2), is increased when using an insufficient spatial resolution. The current is calculated by the Ramo-Shockley theorem and a steady-state is achieved by the periodic injection of individual electrons, represented by minimum uncertainty wave packets. Only the surface roughness is considered; phonons are switched off.

SPWMC simulations rely on the generation of numerical particles with $+$ and $-$ signs [2], generated at a rate in the order of $10^{15}\,\mathrm{s}^{-1}$. Particle annihilation is used to counteract the exponential increase in the number of particles: the phase space is divided into many cells; within each cell particles with opposite signs annihilate each other since their contributions to the calculation of any physical quantity cancel out. The particles remaining after the annihilation are regenerated to represent the pre-annihilation ensemble.

The memory required to represent the phase space grid, on which particles are recorded for annihilation, quickly becomes exorbitant in multi-dimensional simulations with a fine spatial resolution, since the number of cells increases with the power of the dimensionality of the phase space (the resolution also affects the number of $k$-values which must be retained to ensure a unitary Fourier transform). A $30\,\mathrm{nm}\times 30\,\mathrm{nm}$ domain and a three-dimensional $k$-space with a coherence length of $30\,\mathrm{nm}$ results in an array size exceeding $141\,\mathrm{GB}$ at a resolution of $0.2\,\mathrm{nm}$. A distributed-memory (MPI) approach addresses these large memory requirements through a spatial domain decomposition [3]. However, the computational demands of the SPWMC simulator allow it to be run on a typical desktop computer, therefore, its memory demands should also follow suit. Furthermore, a finer resolution also reduces the effectiveness of the annihilation step: there are more cells and each cell is filled by less particles. Thereby, the likelihood of particles with opposite signs to meet and annihilate each other is reduced.

The highlighted problems can be remedied by reducing the spatial resolution of the grid on which the particles are recorded for annihilation; the $k$-values are discretized and remain fixed. The concept is illustrated in Fig. 3. This reduces the memory requirement and increases the effectiveness of the annihilation procedure. To counteract the loss in precision, a statistical fitting of the spatial distribution of the particles in the enlarged spatial cells is performed before annihilation ensues; the obtained distribution is then used to regenerate the particles that remain after the annihilation. Fig. 4 compares the regeneration of particles, annihilated on a coarsened grid, using a uniform distribution and a Gaussian distribution. The former follows the true solution much better than the Gaussian distribution. This is consistent with the observations made in [4]. Both approaches reduce the memory consumption by a factor of 16, however, the Gaussian distribution requires some extra memory and computation to calculate the additional moment. The same holds true for more sophisticated fitting techniques, using more moments of the pre-annihilation distribution, which eradicates the achieved memory reduction.

It is concluded that the debilitating increase in the memory requirements to perform the annihilation step in SPWMC simulations with a fine spatial resolution can be effectively remedied by reducing the spatial resolution of the phase space grid used for recording and performing a statistical fit by calculating the mean position of the particles before the annihilation.

# REFERENCES

[1] J.M. Sellier, M. Nedjalkov, I. Dimov, S. Selberherr, *Decoherence and Time Reversibility: The Role of Randomness at Interfaces*, Journal of Applied Physics, **114**, 174902 (2013).

[2] M. Nedjalkov, P. Schwaha, S. Selberherr, J.M. Sellier and D. Vasileska, *Wigner Quasi-Particle Attributes - An Asymptotic Perspective*, Applied Physics Letters, **102**, 163113 (2013).

[3] P. Ellinghaus, J. Weinbub, M. Nedjalkov, S. Selberherr and I. Dimov, *Distributed-Memory Parallelization of the Wigner Monte Carlo Method Using Spatial Domain Decomposition*, Journal of Computational Electronics, **14**, 151 (2015).

[4] P. Ellinghaus, M. Nedjalkov and S. Selberherr, *Optimized Particle Regeneration Scheme for the Wigner Monte Carlo Method*, Lecture Notes in Computer Science, **8962**, 27 (2015).

[5] S.M. Goodnick, D.K. Ferry, C.W. Wilmsen, Z. Liliental, D. Fathy and O.L. Krivanek, *Surface Roughness at the Si(100)-SiO$_2$ Interface*, Phys. Rev. B, **32**, 8171 (1985).

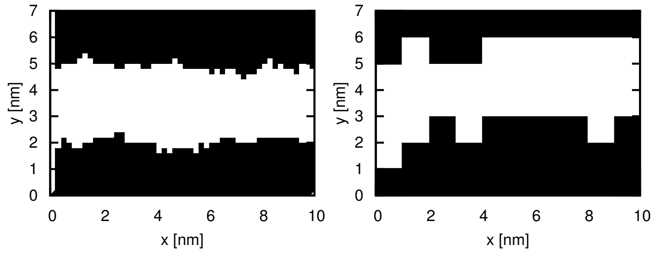

Figure 1. The geometry represents a 3 nm wide silicon channel between two oxide layers (in black). The roughness of the Si/SiO$_2$ interface is characterized by an exponential auto-correlation function with a mean displacement, obtained from experiments in [5], used to perturb the smooth interfaces of the channel. The interface roughness, modeled with identical statistical parameters, results in different effective channel widths when using a 0.2 nm (left) or a 1 nm resolution (right).

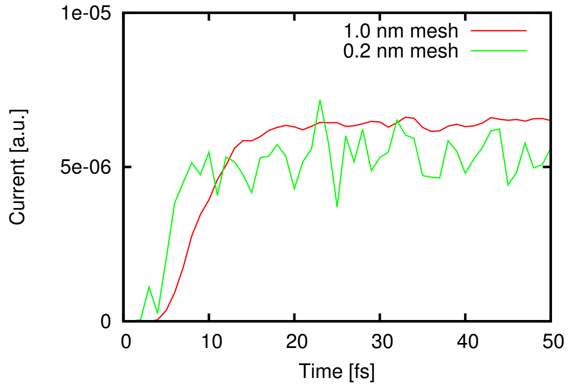

Figure 2. Comparison of the steady-state currents calculated for the geometries in Fig. 1 with a spatial resolution of 0.2 nm and 1.0 nm, show an increase in the latter due to a greater effective channel width. The current increases as the first wave packet is injected into the channel from the left and reaches a steady state once the channel is saturated with particles. The current for the 0.2 nm case appears noisier over the time shown, because it takes longer to saturate the channel with particles on the finer mesh.

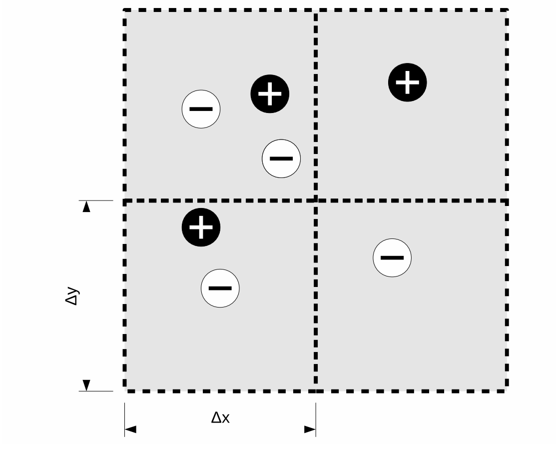

Figure 3. A distribution of + and − particles in four spatial cells (dashed lines). The gray cell, encapsulating all four cells, represents a cell of the coarsened phase-space grid used to perform annihilation. It is enlarged by a factor 2 in both directions, reducing the array size by a factor of four. The effectiveness of annihilation is improved from 3 to only 1 surviving particle.

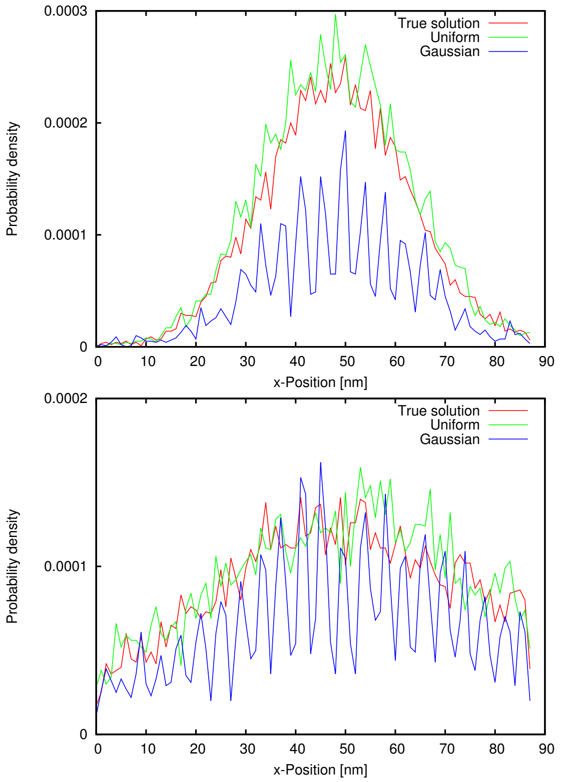

Figure 4. A slice of the two-dimensional probability density of a wave packet, evolving freely in a domain with a spatial resolution of 0.25 nm, after 40 (top) and 80 (bottom) forced annihilation steps. The annihilation is performed on a coarsened grid with a 1 nm resolution and the particles are regenerated using uniform and Gaussian distributions. The 'true solution' – the evolution when the annihilation step is omitted – is followed the best when particles are regenerated by a uniform distribution.