

additional phase despite that in both cases there are no fields. This effect is analyzed from a phase space perspective with the help of the Wigner formulation of quantum mechanics. Simulation results show that the effect is revealed by the dependence of the interference part of the entangled electron state on the potential value. It is discussed, how the destruction of this interference part recovers the classical behavior.

Sensitivity Analysis of Checkpointing Strategies for Multimemetic Algorithms on Unstable Complex Networks

R. Nogueras, C. Cotta

The use of dynamic decentralized computational platforms such as, e.g., peer-to-peer networks, is becoming an increasingly popular option to gain access to vast computing resources. Making an effective use of these resources requires algorithms adapted to such a changing environment, being resilient to resource volatility. We consider the use of a variant of evolutionary algorithms endowed with a classical fault-tolerance technique, namely the creation of checkpoints in a safe external storage. We analyze the sensitivity of this approach on different kind of networks (scale-free and small-world) and under different volatility scenarios. We observe that while this strategy is robust under low volatility conditions, in cases of severe volatility performance degrades sharply unless a high checkpoint frequency is used. This suggest that other fault-tolerance strategies are required in these situations.

Spin Lifetime in MOSFETs: A High Performance Computing Approach

D. Osintsev, J. Ghosh, V. Sverdlov, J. Weinbub, S. Selberherr

We study spin properties in ultra-scaled silicon MOSFETs. To evaluate the spin relaxation time, a multi-dimensional integral over the energy and different directions of the wave vectors before and after scattering must be taken. The inner integrals over before- and after-scattering directions at a fixed energy require at least 1000 points each. The energy integration requires around 1400 points with a uniform grid. Thus, the scattering matrix elements and the Jacobian (the derivative of the dispersion energy over the wave vector) must be calculated numerically around a billion times. To compute the matrix elements, the eigenfunction problems for the 4×4 Hamiltonian matrix must be solved for the two wave vectors before and after scattering for a broad range of parameters, which makes the numerical spin relaxation time calculation prohibitively expensive. Indeed, when utilizing a standard adaptive integration technique we found that a month of calculations on 20 cores, or 15000

core-hours total, was required to evaluate a single data point of the relaxation time as a function of stress. This is due to extensive swapping of intermediary data, and an approach which uses cache efficiently must be developed.

Parallelization has been implemented by using the message passing interface library. In order to make the calculation efficient the Boost and GSL libraries, augmented with the cache memory technique, have been used. This approach has been tested on 416 cores and requires only around 40 minutes for a single relaxation time data point (around 300 core-hours). We have further improved the calculation efficiency and scalability to make calculations possible for different input parameters of thin-body silicon films.

We first use the approach to study the electron mobility enhancement in uniaxially stressed silicon channels. The electron mobility enhancement by a factor of two is obtained, in agreement with earlier findings. In contrast, for the same stress values the spin lifetime is boosted by an order of magnitude. The physical reasons behind the giant spin lifetime enhancement with strain are revealed.

High Performance Tools for Sensitivity Analysis with Application in the Air Pollution Modelling

Tz. Ostromsky, I. Dimov, V. Alexandrov, Z. Zlatev

Sensitivity analysis is a way to estimate the uncertainty of the output of a model with respect to the different sources of uncertainty in the input data. Such a study plays an important role in mathematical modelling, especially for reliability analysis of the results of complex nonlinear models. Various sensitivity analysis techniques have been developed in the last 3 decades. Among the quantitative methods, variance-based methods are most common. These are based on the idea to evaluate how the variance of (a group of) inputs contributes to the variance of model output.

We developed a computationally efficient 3-stage method for global sensitivity analysis of a large-scale air pollution model, the Danish Eulerian Model (DEM). This powerful model consists of several modules (including some non-linear). There is a number of uncertain internal parameters, especially in the chemistry-emission submodel, which are subject to our quantitative sensitivity study. Efficient Monte Carlo and quasi-Monte Carlo algorithms based on Sobol sequences are used in this study.

A large number of numerical experiments with the target model must be carried out in order to collect the necessary input data for the particular sensitivity study. Therefore we created an efficient high performance implementation (called SA-DEM), based on the parallel MPI version of the package UNI-DEM. A large number of numerical experiments were carried out with SA-DEM on the Bulgarian IBM Blue Gene/P (currently the most powerful parallel supercomputer in Bulgaria). Even this powerful machine has some problems with the storage when SA-DEM must be run with the refined (480 x 480) grid version of the domain. The code was implemented with some improvements and extended abilities on the IBM MareNostrum III at BSC