Numerical Modeling of Groundwater Depletion and Restoration Strategies in Coastal California

T. Russo

Numerical modeling applications in hydrogeology range from pore scale to global simulations, and help quantify fluid and solute transport dynamics in variably saturated, multi-permeability, and multiphase systems. Simulations of flow are essential for addressing issues of fundamental hydrologic science, and even more so for developing and testing management or remediation strategies. Numerical modeling can be used to explore and evaluate management options without expending the cost and time required by field testing. We present a brief overview of numerical modeling in hydrology, followed by a case study of a severely overdrafted coastal basin in California, USA. A finite difference fluid transport model was used to evaluate the efficacy of groundwater restoration strategies, specifically managed aquifer recharge (MAR) impact on groundwater level recovery and reduction of seawater intrusion into the local aquifers. First, we developed MAR project placement scenarios based on an analysis of surface and subsurface hydrologic properties and conditions, using a geographic information system (GIS). Second, we assessed the hydrologic impact of potential MAR placement and operating scenarios. For the region evaluated in this study, GIS results suggest that about 7% (15 km^2) of the basin may be highly suitable for MAR. Numerical modeling results suggest that simulated MAR projects placed near the coast help to reduce seawater intrusion more rapidly, but these projects also result in increased groundwater flows to the ocean (i.e. applied MAR water inefficiency). In contrast, projects placed farther inland result in more long-term reduction in seawater intrusion and less groundwater flowing to the ocean. This work shows how numerical modeling can assist with regional water supply planning, including evaluation of options for enhancing groundwater resources.

Monte Carlo Particles in Quantum Wires: Effects of the Confinement

T. Sadi, E. Towie, M. Nedjalkov, A. Asenov, S. Selberherr

The electrical performance of modern quantum wire based devices, having active regions with dimensions comparable to the physical spread of the electrons inside the structures, is strongly influenced by quantum effects. Confined electrons experience frequent reflections from the wire walls to move along a one-dimensional (1D) transport direction, and are affected by complicated microscopic quantum processes which determine their evolution. In contrast to electrons in 3D structures, carriers in 1D systems do not have well-defined momenta in the 2D plane of confinement. Moreover, energy quantization giving rise to 2D multi-subbands occurs. These effects strongly

modify the scattering mechanisms, which critically affects the transport properties of Monte Carlo solutions of the Boltzmann Transport Equation (BTE) for device modeling. A full first-principles based mathematical derivation of the scattering rate models for each mechanism is needed, which considers the solution of the stationary Schrodinger equation in the 2D plane. The implementation of these advanced mathematical models for scattering rates is necessary for studying transport in confined nanostructures, which presents a significant challenge for most of the well established 3D Monte Carlo approaches for device simulation.

We have developed 1D multi-subband (1DMS) models for phonon, surface roughness, ionized impurity, and alloy disorder scattering for electrons, needed for the Monte Carlo (MC) approach for a rigorous simulation of quantum wire devices. The scattering models have been incorporated within a 1DMS Monte Carlo (1DMSMC) simulator. We demonstrate the effect of the scattering mechanisms, material properties, and geometrical features on both the low- and high-field electron mobility and velocity. The importance of 1DMS scattering models which correctly include quantum confinement is shown by comparing 1DMSMC simulation results with 3D MC calculations using conventional bulk scattering models. 1DMS scattering models enable a reliable prediction of the performance of quantum wire based devices.

Metric Sub-Regularity and High Order Time-Discretization of Linear-Quadratic Problems with Bang-Bang Controls

T. Scarinci, V. M. Veliov

The talk will present a new discrete approximation scheme for solving optimal control problems for linear systems, where a Lagrange type objective function is to be minimized and the optimal control is of bang-bang type. The novelty is in that the error estimate is of higher order with respect to the mesh size than the known discretizations schemes (generically, it is of second order). The scheme is based on a truncated Volterra-Fliess expansion and a new result about metric sub-regularity of the associated system of necessary optimality conditions. Numerical evidence of the advantage of the proposed discretization will be provided.

Stress-Velocitiy Mixed Least-Squares FEMs for the Time-Dependent Incompressible Navier-Stokes Equations

A. Schwarz, C. Nisters, S. Averweg, J. Schröder

In this contribution mixed least-squares finite element methods (LSFEMs) for the time-dependent incompressible Navier-Stokes equations are proposed and investigated with respect to accuracy and efficiency. Starting from the well-known stress-