ERCIM "Alain Bensoussan" Fellowship Scientific Report

Fellow: Markus Brunk
Visited Location : NTNU Trondheim, Department of mathematical sciences
Duration of Visit: 02.04.2008 – 01.04.2009

I - Scientific activity

Main focus of the scientific activity was positivity preserving discretization of the transient semiconductor drift-diffusion and the semiconductor energy-transport equations. We showed that discretization of the transient drift-diffusion equations by the vertical method of lines, using mixed hybrid finite elements leads to differential-algebraic equations with index of at most one. We showed that the solution of this DAE is non-negative, as long as non-negative boundary and initial conditions are applied. Moreover we showed that the applied mixed finite element scheme, namely Marini-Pietra FEM, is optimal in the sense that it ensures positivity, allows for good current regularity and the resulting system is cheap to solve. Not even a mixed-hybrid Petrov-Galerkin approach could fulfill these conditions.
Finally, we suggested a splitting algorithm based on exponential integration and Rosenbrock methods that allows to increase the step size restriction for positivity preservation when integrating the semi-discretized system. For backward biased *pn*-junction diodes, this algorithm allows to speed up (positivity-preserving) simulation, when the splitting-algorithm is coupled to the well known Gummel-algorithm. The publication of those results is in progress.

Besides that we considered the coupling of one-dimensional energy-transport model for semiconductor devices with circuit equations resulting from modified nodal analysis (MNA). We considered the index of the DAE resulting from the coupling of MNA-equations and space discretized energy-transprt equations, where mixed hybrid FEM has been applied for space discretization. We showed, that in this case similar index results are valid as in case of the simpler drift-diffusion model coupled to the MNA equations. The publication of these results is still in progress.

The last branch of the scientific work within this year was dedicated to the thermal-electric modeling of electric circuits containing semiconductor devices. In this framework, I continued work I started during my PhD. Finally, a model with new considereation of thermal effects in semiconductor devices has been derived and coupled to network equations. These results have been published partially in the proceedings of SCEE 2008 and are partially submitted for publication to a scientific journal.

II- Publication(s) during your fellowship

1. M. Brunk and A. Jüngel. *Self-heating in a coupled thermal-electric circuit-device model.* Submitted for publication.

   Abstract:
   The self-heating of a coupled thermo-electric circuit-semiconductor system is modeled and numerically simulated. The system consists of semiconductor devices, an electric network with resistors, capacitors, inductors, and voltage sources, and a thermal network. The flow of the charge carriers is described by the energy-transport equations coupled to a heat equation for the lattice temperature. The electric circuit is modeled by the network equations from modified nodal analysis coupled to a thermal network describing the evolution of the temperatures in the lumped and distributed circuit elements. The three subsystems are coupled through thermo-electric, electric circuit-device, and thermal network-device interface conditions. The resulting system of nonlinear partial differential-algebraic equations is discretized in time by the 2-stage backward difference formula and in space by a mixed finite-element method. Numerical simulations of a one-dimensional ballistic diode and a frequency multiplier circuit containing a *pn*-junction diode illustrate the heating of the semiconductor device and circuit resistors.

2. M. Brunk and A. Jüngel. *Heating of semiconductor devices in electric circuits.* To appear in Proceedings to SCEE 2008.

   Abstract:
   Thermal effects in a coupled circuit-device system are modeled and numerically simulated. The circuit equations arise from modified nodal analysis. The transport in the semiconductor devices is modeled by the energy-transport equations for the electrons and the drift-diffusion equations for the holes, coupled to the Poisson equation for the electric potential. The lattice temperature is described by a heat equation with a heat source including energy relaxation heat, recombination heat, hole Joule heating, and radiation. The circuit-device model is coupled to a thermal network. The resulting system of nonlinear partial differential-algebraic equations is discretized in time using backward difference formulas and in space using (mixed) finite elements. Heating effects from numerical simulations in a *pn*-junction diode and a clipper circuit are presented.

3. M. Brunk and A. Kværnø. *Positivity preserving discretization of time dependent semiconductor model equations.* In preparation.

   Abstract:
   Positivity preserving discretization of the semiconductor drift-diffusion equations are considered. The drift-diffusion equations are spatially discretized by mixed hybrid finite elements. It is shown that this leads to a positive ODE or DAE system with index of at most one. For time discretization a second order splitting technique based on a combination of explicit exponential integration and implicit one-step methods is proposed. The technique allows for positivity preservation with larger step sizes than the corresponding one-step methods of higher order. A algorithm is presented coupling the proposed splitting technique with the Gummel iteration scheme for semiconductor equations allowing for efficient positivity preserving device simulation. Numerical results for a one-dimensional *pn*-diode are given, showing that the proposed scheme allows for runtime acceleration

III -Attended Seminars, Workshops, and Conferences

08.05.2008: Seminar of numerics workgroup at NTNU
Active part: Oral presentation concerning ongoing research and research plan for the exchange programme

28.09.2008 – 03.10.2008: SCEE
Conference on Scientific Computing in Electrical Engineering in Espoo, Finland.
Active part: Poster presentation

03.03.2009 – 06.03.2009: MaGIC
Manifolds and Geometric Integration Colloquia at Hornsjø, Lillehammer, Norway.
Active part: Oral presentation

10.03.2009: Student seminar at host institute
Active part: Oral presentation for students

IV – Research Exchange Programme (12 month scheme)

20.10.2008 – 29.20.2008: CWI
Centrum Wiskunde & Informatica, Amsterdam, Netherlands
Contact persons: W. Hundsdorfer & J. Verwer

Collaboration:

- Intensive discussion with W. Hundsdorfer and J. Verwer about positivity preserving integration of ODEs
- Succesful derivation of positive linear systems by discretizting the semiconductor drift-diffusion equations
- Discussions with W. Hundsdorfer about effective numerical coupling of advection-diffusion equations with electric network equations

11.12.2008 – 19.12.2008 :
Wolfgang Pauli Institute Vienna, Austria
Contact persons: C. Schmeiser, A. Jüngel

Collaboration:

- Discussions about modeling of thermal effects in semiconductor devices and thermal simulation of electric networks.
- Discussion about positivity preserving discretization for semiconductor energy-transport equations
- Work on common publication