# Dr. Gerhard Klimeck

Purdue University, School of Electrical and Computer Engineering
465 Northwestern Ave., West Lafayette, IN 47907

Email: gekco\_nospam@purdue.edu

#### **OBJECTIVE**

Provide leadership to the Network for Computational Nanotechnology as a Technical Director and continue nanoelectronic research, high performance computing, and software engineering at Purdue University. Serve as a link between JPL and Purdue in these areas of research.

#### **EDUCATION**

**Ph.D., Electrical Engineering,** Purdue University, GPA: 4.00/4.00

1994

Thesis: Electron-Electron and Electron-Phonon Interactions in Quantum Transport.

Advisor: Professor Supriyo Datta

Dipl. Ing., Electrical Engineering, Ruhr University Bochum, Germany (equiv. M.S.E.E.)

1990

GPA: 5.97/6.00 (converted from German system), Class Rank 2/167

Thesis: Laser Noise Induced Intensity Fluctuations in an Optical Interferometer.

Advisor: Professor Daniel S. Elliott, Purdue.

Engineering Co-op program with Thyssen Mechanical Engineering, RWE, and Siemens AG.

#### **EMPLOYMENT**

Purdue University, School of Electrical and Computer Engineering

Professor, Technical Director of the NSF Network for Computational Nanotechnology 12/03-present

**Jet Propulsion Laboratory,** Applied Cluster Computing Technology / High Perf. Computing Group Principal Member of Technical Staff 9/01-present Technical Group Supervisor of the Applied Cluster Computing Technology Group 4/02-12/03

Senior Member of Technical Staff

2/98-9/01

- Development of an atomistic nanoelectronic modeling and simulation tool
- Development of a genetic algorithm based optimization and synthesis tool
- Parallelization of Mars imaging software

**Texas Instruments Incorporated**, Corporate Research and Development (transitioned to **Raytheon TI Systems**, Applied Research Laboratories 8/97).

9/95-2/98

Member of Technical Staff - Nanoelectronics Research Group

- Development of the Nanoelectronic Modeling software (NEMO) including theory, algorithms, user-interface, implementation, verification, documentation and delivery.
- Project Management: responsible for proposal development, project planning, labor scheduling, agency interaction, monthly reports to NRO/NSA, and quarterly reviews.

University of Texas at Dallas, School of Engineering

5/97-8/97

Lecturer. Teaching "Advanced Semiconductor Device Theory", graduate level course with about 18 students, primary text book: S. Datta, "Quantum Phenomena"

University of Texas at Dallas, School of Engineering

2/94-9/95

Post-doctoral Research Associate - Supervisor: Professor William R. Frensley

• Prototype development of NEMO. Consultant to Texas Instruments Corporate Research and Development. Provided grid generation algorithms for DARPA/ULTRA.

Purdue University, School of Engineering

9/90-1/94

Research Assistant - Supervisor: Professor Supriyo Datta

Ruhr-University Bochum, School of Engineering

2/88-8/88

Research Assistant - Supervisor: Professor Eckhard Kneller

## **SELECTED HONORS**

- Author of, or major contributor to, successful research proposals worth over \$2.7M.
- Co/Author of over 321 publications: 51 journal, 46 proceedings, 158 conf., 66 seminars/reviews.
- JPL Dr. Edward Stone Award for Outstanding Research Publication 2002.
- US Patent 6,490,193: "Method and System for Generating a Memory Cell".
- Texas Instruments Award for timely delivery of the Phase II NEMO software.
- DARPA Award to Raytheon-TI Systems: Sustained Excellence by a Performer in FY97.
- Scholarships: Purdue Fee Remission Award, National Science Foundation of Germany.
- Member of ηκν ΕΕ Honor Society, τβπ Engineering Honor Society, IEEE and APS.
- Tae Kwon Do 2<sup>nd</sup> degree black belt and member of the Caltech Soccer Club.

## **PUBLICATION SUMMARY**

• The following two pages highlight my research activities with references to publications.

•	Publication count:	total		total
	- Peer reviewed journals:	51	- Technical Reports:	20
	- Peer reviewed proceedings:	46	- Invited Seminars:	37
	- Invited conference papers:	41	- Technical Program Reviews	29
	- Contributed conference papers:	117	C	

• Citation count in Database of Institute for Scientific Information: 425 (approx. >300 by others).

# RESEARCH HIGHLIGHTS (WORK PERFORMED AT JPL)

- Atomistic Nanoelectronic Modeling in 3-D Developed a bottom-up nanoelectronic modeling tool for the analysis of the electronic structure in a nano-scale system based on the representation of each individual atom in the structure. The simulator enables the analysis of electronic structure and optical response in a variety of crystal structures and material systems. The first structures analyzed were quantum dots. General nanoscale electronics problems such as interface roughness, randomized impurities and radiation effects are to be tackled as well. Demonstrated the simulation of a system as large as 32 million atoms. Parallelized the simulator on a Linux-based Beowulf system. Studied effects due to atomic alloy disorder and interface interdiffusion in quantum dots [33, 36, 39, I21-I31]. Optimized material parameters resulted in good experimental agreement for optical transitions in colloidal quantum dots [33,38].
- Parallelization of Mars Imaging Software Converted existing serial Mars imaging software (e.g. mosaic generation from many images, left/right eye correlation for two images) to efficient parallel code. Hardware: COTS Linux-based Pentium III cluster (Beowulf) using MPI. Achieved time reductions from original baseline of 90 minutes to 3 minutes (mosaic software) and 90 minutes to 6 minutes (correlator). This acceleration enables fast feedback (near real-time) to mars rover control [P27, P30].
- Genetic Algorithm-Based Optimization and Synthesis Developed an optimization and synthesis tool based on a massively parallel genetic algorithm (GA) and incorporated various high-level simulation tools into the toolbox.
  - Material Science: Performed parameterization of tight banding bandstructure models to achieve the proper representation of basic material properties such as bandgaps and effective masses. NEMO+GA [28, 29, 36, 37].
  - Electron device synthesis: Solved the inverse resonant tunneling diode design problem: what is the structure that will generate a particular current-voltage characteristic? NEMO+GA [P18, P20].
  - Circuit synthesis: Enabled a GA based circuit configuration on an FPGA to achieve a Gaussian pulse response. SPICE + GA [P22, P23].
  - Optical filter synthesis: Optimized a pattern on a frequency selective surface to achieve optimal transmission and reflection. [P22, P23].
- **High Performance Computing Extensions to NEMO 1-D** Parallelized existing NEMO 1-D software on various simultaneous levels using MPI. Ported parallel code to SGI and Beowulf massively parallel machines. Achieved unprecedented high fidelity resolution of carrier transport through 1-D heterostructures and uncovered unintuitive quantum transport phenomena [30, 31, 32, 34, 40].
- **Tight-Binding Model Theory** Collaborated with Prof. Tim Boykin on the fundamental understanding of tight binding models and their applications to quantum transport simulations [25-29].

# RESEARCH HIGHLIGHTS (WORK PERFORMED PRIOR TO JPL)

- Comprehensive Quantum Electron Transport Principal designer and developer of the NEMO software. NEMO is the world's first comprehensive 1-D quantum electron transport simulator including effects due to charging, multiple bands and scattering. NEMO has shown predictive capabilities useful for devices design and analysis. The world's first high-bias quantum mechanical, simulations of scattering enhanced charging and charge self-consistency of holes and electrons [9-24,P4-P17] for RTDs were generated.
- **High Bias Coulomb Blockade** Initiated analysis of high bias transport in quantum dots. Key investigator of Coulomb blockade at Purdue University [8,P1].
- Linear Response of Coupled Quantum Dots Proposed experiment on conductance spectroscopy in coupled quantum dots and analyzed experimental feasibility [6,7]. This work is cited over 70 times.
- Scattering Studied the scattering enhanced valley current in RTDs [4,5,9-24,P4-P17].
- 2-D Linear Response Analyzed anomalous Quantum Hall Effect in 2-D electron gas system. [3].
- Laser Noise Experiments Implemented high frequency (200MHz) laser amplitude modulation circuitry. Developed laser stability controller (15 kHz) using an external resonance cavity. Measured the propagation of laser noise through optical systems. Calculated and measured higher order, non-linear laser noise fluctuations [1,2].
- Thin Film Deposition Analyzed the experimental feasibility of a novel fast thin film deposition process. Fabricated first clean metallic films (senior project).

## PROGRAMMING EXPERIENCE

- **Software Project Management** NEMO is a simulation tool consisting of about 250,000 lines of code. Tackled issues of software design, documentation, release and maintenance.
- **Hybrid Language Design** Developed hybrid C, F77 and F90 code which allows the utilization of the flexibility of object oriented C data structures and vectorization capabilities of F77 and F90.
- **Software Documentation** Invented a software documentation tool that allows for a close connection of the development software and its structural documentation. Pseudo code and code are kept in one file but can be presented in a user friendly, interactive form.
- **Numerical Methods** Solutions of large, sparse systems of equations, Eigen-value and Eigen-vector analysis of large systems, program vectorization.
- **Software Release** Released NEMO code at Raytheon with 3,000 pages of documentation, consisting of User's Guide, Theory Guide and Developer's Guide. At Purdue co-authored and released 2 Purdue University simulation packages: SQUALID-2D and QUEST. Developed QUEST User's Manual and Tutorial [T1,T2].
- Systems Linux, HP-9000, SUN, IBM-RISC, SGI, IBM SP2, Ardent, and GOULD, MAC, MS.

## TEACHING EXPERIENCE

- Lecturer at University of Texas at Dallas, full semester night time course to ~18 masters and Ph.D. students, "Advanced Semiconductor Device Theory", Text book primarily used: S. Datta, Quantum Phenomena.
- Substitute teaching for Professor Supriyo Datta at Purdue University.
- Mentored Post-Doctoral Researchers and summer students (see professional services section).
- National Research Council Advisor.
- Conducted user training sessions for the NEMO software.
- Instructor of the Purdue Jido Kwan Tae Kwon Do club (3 years).

## PERSONAL / ACADEMIC ACHIEVEMENTS

- 10/1987 Best in Prediploma Class in Electrical Engineering at the Ruhr University Bochum.
- 10/1990 Second Best in Diploma Class in Electrical Engineering at the Ruhr University Bochum.
- 01/1994 Defended Ph.D. thesis at Purdue University with GPA of 4.00/4.00.
- 03/1992 1<sup>st</sup> degree black belt, World Tae Kwon Do Federation, South Korea.
- 05/1993 2<sup>nd</sup> degree black belt, World Tae Kwon Do Federation, South Korea.

## **SCHOLARSHIPS**

- 04/1987-09/1990 Friedrich Ebert Stiftung, Begabtenförderung, Germany Full ride scholarship for gifted students providing monthly stipend and book expenses (there is no tuition at public German Universities).
- 04/1987 RWE Industrial Scholarship
  Three year scholarship providing stipend for students selected by the Institute of Power Electronics at the University of Bochum.
- 02/1988-09/1990 Studienstiftung des Deutschen Volkes, Begabtenförderung Most prestigious German scholarship for gifted students from the equivalent of the US National Science Foundation.
- 08/1988-05/1989 Deutscher Akademischer Austauschdienst (DAAD), Integriertes Auslandsstudium German Academic Exchange Service Scholarship for support of exchange program participation between Bochum and Purdue, providing travel expenses, living-abroad supplement, and US health insurance.
- 08/1988-05/1989 Purdue University Fee Remission Award.
- 08/1989-09/1990 Friedrich Ebert Stiftung, Begabtenförderung Scholarship expansion for tuition and additional living-abroad supplement.

## RESEARCH PROPOSAL AWARDS

- 1999, SBIR Phase I Award, ONR, \$100k, 6 months, "An Advanced CAD Tool for Quantum Device Simulation", PI: Phillip Stout, CRFDR Corporation, Co-I Gerhard Klimeck.
- 12/2001, JPL Directors Research and Discretionary Fund (DRDF), \$100k, 18 months, "Nanoelectronic and Nanomagnetic Devices for Revolutionary Computing and Sensor Applications", PI: Gerhard Klimeck, participating: Fabiano Oyafuso (JPL).
- 03/2002, JPL Internal Research and Development, \$343k, 6 months, "Evolutionary Computing Technologies for Space Systems", PI: Richard Terrile, Co-PI: Gerhard Klimeck, and others.
- 03/2002, NSA/ARDA, \$900k, 3 years, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", PI: Gerhard Klimeck, participating: Fabiano Oyafuso (JPL), Timothy Boykin (U. Alabama Huntsville).
- 07/2002, ONR, \$680k, 3 years, "Atomistic 3-D Nanoelectronic Modeling (NEMO) for Electron Transport in Realistic Nano-Scale Devices", PI: Gerhard Klimeck, participating: Fabiano Oyafuso (JPL), Supriyo Datta (Purdue Univ.).
- 07/2002, SRC, \$468k, years, (JPL collaborator only no funds exchanged), "Study of Mobility Degradation and Detailed Structure of Si/high-k Interfaces including Dopant Segregation Using AIDA-TEM (Ab-initio Interface Defect detection by Analytic Transmission Electron Microscopy)", PI: Wolfgang Windl (Ohio State U), Co-PIs: Gerd Duscher (North Carolina State U), Maria Merlyne De Souza (De Montfort U).
- 09/2002, NSF Nano Science Center, \$12,500k over 5 years, (JPL is government collaborator no funds exchanged), "Network for Computational Nanotechnology", PI: Mark Lundstrom.
- 10/2002, JPL Internal Research and Development, \$624k, 12 months, "Evolutionary Computing Technologies for Space Systems", PI: Richard Terrile, Co-PI: Gerhard Klimeck, and others.
- 04/2003, JPL Internal R&TD, \$30k, 3 months, "Simulation of hydrogen sensors with Pd nanowires", PI: Paul von Allmen, Co-I: Seungwon Lee and Gerhard Klimeck.

## **AWARDS / RECOGNITIONS**

- 10/1987 Siemens circle of selected, highly qualified students in Engineering and Sciences. Support for a one-week seminar, science books, selected internships and senior and thesis projects.
- 12/1988 Purdue dean's list.
- 1989 HKN Electrical engineering honor society.
- 1989 TBP Engineering honor society.
- 02/1990 Permanent Member of the most prestigious German Science Foundation, Permanentes Mitglied der Studienstiftung des Deutschen Volkes.
- 03/1991 Foundation for German Science, Prize for the especially fast and very successful completion of studies.
  - Stifterverband für die Deutsche Wissenschaft, Preis für ein in besonders kurzer Zeit sehr erfolgreich abgeschlossenes Studium.
- 1992 Best student presentation in Purdue EE Industry Initiative Workshop.
- 07/1995 Recognition of my US PhD degree within the German official title system by the Department of Science and Research.

  Ministerium für Wissenschaft und Forschung des Landes NRW: Zustimmung zur Führung eines ausländischen Grades: Ph.D. (USA) oder Dr. (USA).
- 10/1996 Texas Instruments Award, Citation: Gerhard Klimeck is recognized for outstanding achievement in the development and demonstration of quantum device design tools. His leadership in developing computer code and documentation for NEMO, a world class device modeling program exceeded customer requirements and helped win follow-on contract. Due to this effort, TI has strengthened its competitive position in nanoelectronics and is viewed by our customers as the industry leader in the development of quantum design tools.
- 1997 DARPA, Ultra Dense, Ultra Fast Computing Components, Award to Raytheon-TI Systems: Sustained Excellence by a Performer in Fiscal Year 1997.
- 2002 JPL, Dr. Edward Stone Award for Outstanding Research Publication, Citation: This paper represents a milestone publication for JPL's entry into the field of nanoelectronic device modeling and simulation for future NASA missions. It is also of value to the international semiconductor industry community.
- 2003 NASA Tech Brief Award: NTR no. 30520, "Nanoelectronic Modeling 3-D (NEMO 3-D) Upgrade"
- 2003 NASA Space Act Award: NPO no. 30520, "Nanoelectronic Modeling 3-D (NEMO 3-D) Upgrade"
- 2004 NASA Tech Brief Award: for NTR no 30842: "WIGLAF (A Web Interface Generator and Legacy Application Façade)."

# **PATENT**

• US Patent 6,490,193: "Method and System for Generating a Memory Cell", Paul van der Wagt and Gerhard Klimeck, work performed at Texas Instruments and Raytheon TI Systems.

# TECHNICAL GROUP SUPERVISOR (APPLIED CLUSTER COMPUTING TECHNOLOGY GROUP):

- Supervision of 11 computer science, electrical engineering and physics professionals (6 Ph.D., 3 master, 2 bachelor) and one National Research Council post-doc. Responsibilities include:
  - Technical quality of the work produced in the group.
  - Mentoring of the professional careers of the group members (promotions, salary management).
  - Direct interface between two axes of management at JPL: 1) line management (people) and 2) project management (tasks, money). Matching of technical expertise with project requirements.
  - Enforcement of JPL policies.
  - Equipment purchase responsibilities of up to \$150,000.
- Direct technical involvement in a diverse set of tasks:
  - Nanoelectronic modeling for quantum computing gates.
  - Nanoelectronic modeling development of numerically tractable open boundary conditions.
  - Spintronic modeling.
  - Evolvable computing (optimization and synthesis using genetic algorithms).
  - Java and portlet-based graphical user interface development.
  - Cluster computing technologies applied to science applications such as optical as well as synthetic aperture radar (SAR) image processing.
  - Adaptive, unstructured mesh refinement.
  - COTS-based on-board image processing.
  - XML-based non relational database design for project descriptions and evaluations.

# PROGRAM COMMITTEE, CONFERENCE PREPARATION, SESSION CHAIR

- Program Committee, 27th international Symposium on Compound Semiconductors (ISCS), IEEE, (2000), Monterey, CA, Oct 2-5, 2000.
- Session Moderator, Quantum Transport, Advanced Research Workshop on Quantum Transport in Semiconductors, Maratea, Italy, June 17-22, 2001.
- Program Committee, Session Chair, Nanoelectronics Session, Nanospace 2002, Galveston, TX, June 24-28, 2002.
- Session Chair, Superlattices and Resonant Tunneling Structures, March Meeting of American Physical Society, March 16-21, Austin, TX (2003).
- Program Committee, 2nd International Workshop on Quantum Dots for Quantum Computing and Classical Size Effect Circuits, University of Notre Dame, August 7-9, 2003.

# JOURNAL REVIEWER / REFEREE

- Physical Review B and Physical Review Letters
- physica status solidi b
- Superlattices and Microstructures
- IEEE Transactions on Electron Devices, IEEE Transactions on Nanotechnology
- Journal for Computational Electronics
- VLSI Design

## SCIENTIFIC MENTOR / ADVISOR

- Advisor for the National Research Council. Advisor to Dr. Olga Lazarenkova at JPL. 01/03-present.
- Post-Doc mentor / collaborator to Dr. Paul Sotirelis, Texas Instruments, 09/96-01/98.
- Mentor to several summer students in a governmental or industrial laboratory environment:
  - Daniela Francovicchio, Texas Instruments, UT Dallas, 08/95-12/95, NEMO benchmarking.
  - Mukund Swaminathan, Texas Instruments, 06/97-01/98, NEMO software development.
  - William McMahon, Texas Instruments, 05/97-08/97, NEMO database development.
  - Kalen Jordan, JPL, academic part time, 05/01-08/01, Java interface development.
  - Hook Hua, academic part time, 04/02-02/03, Java/XML interface development.
  - Lei Pan, academic part time, 08/03-present, parallel application development.

#### **PUBLICATION SUMMARY**

Publication count:	total		total
- Peer reviewed journals:	51	- Technical Reports:	20
- Peer reviewed proceedings:	46	- Invited Seminars:	37
- Invited conference papers:	41	- Technical Program Reviews	29
- Contributed conference papers:	117	C	

• Citation count in Database of Institute for Scientific Information: 425 (approx. >300 by others)

# SUBMITTED JOURNAL PUBLICATIONS

- [zzz] Seungwon Lee, Paul von Allmen, Fabiano Oyafuso, Gerhard Klimeck, K. Birgitta Whaley, "Effect of electron-nuclear spin interactions on electron-spin qubits localized in self-assembled quantum dots", submitted to Phys. Rev. B. (2004).
- [zzz] Timothy B. Boykin, Gerhard Klimeck, M. A. Eriksson, Mark Friesen, S. N. Coppersmith, Paul von Allmen, Fabiano Oyafuso, and Seungwon Lee, "Analytic solution methods for tight-binding models of quantum-confined heterostructures", submitted to Phys. Rev. B. (2004).
- [zzz] Jeremy Green, Timothy B. Boykin, Corrie D. Farmer, Michel Garcia, Charles N. Ironside, Gerhard Klimeck, Roger Lake, and Colin R. Stanley, "Quantum cascade laser gain medium modeling using a second-nearest-neighbor sp3s\* tight-binding model", submitted to IEEE J. of Quantum Electronics (2004).
- [y] Paul von Allmen, Gerhard Klimeck, Fabiano Oyafuso, Nick Rizzo, Brad Engel, Herb Goronkin, "Interplay of spin precession and spin diffusion across a semiconductor interface", submitted to Appl. Phys. Lett. (2003).
- [z] Carl L. Garner, Christian Ringhofer, Gerhard Klimeck, and R. Chris Bowen, "Smooth Quantum Hydrodynamic Model vs. NEMO Simulation of a Resonant Tunneling Diode", submitted to Journal of Computational Electronics, 2002.

# JOURNAL PUBLICATIONS (WORK PERFORMED AT JPL)

- [51] Timothy B. Boykin and Gerhard Klimeck, "The discretized Schrödinger equation and simple models for semiconductor quantum wells", accepted in Eur. J. of Phys. (2004).
- [50] Olga L. Lazarenkova, Paul von Allmen, Fabiano Oyafuso, Seungwon Lee, and Gerhard Klimeck, "Atomistic model for the simulation of acoustical phonons, strain distribution, and Grüneisen coefficients in zinc-blende semiconductors", accepted for publication in Superlattices and Microstructures (2004).
- [49] Seungwon Lee, Fabiano Oyafuso, Paul von Allmen, and Gerhard Klimeck, "Boundary conditions for the electronic structure of finite-extent, embedded semiconductor nanostructures with empirical tight-binding model", Phys. Rev. B 69, 045316 (2004).
- [48] Timothy B. Boykin, Gerhard Klimeck, and Fabiano Oyafuso, "Valence band effective mass expressions in the sp3d5s\* empirical tight-binding model applied to a new Si and Ge parameterization", Phys. Rev. B. 69, 115201, No 11 (2004)
- [47] Timothy B. Boykin, Gerhard Klimeck, Mark Eriksson, Mark Friesen, S. N. Coppersmith, Paul von Allmen, Fabiano Oyafuso, and Seungwon Lee, "Valley splitting in strained silicon quantum wells", accepted for publication in Applied Physics Letters.
- [46] Gerhard Klimeck, "Quantum and semi-classical transport in RTDs in NEMO 1-D", accepted for publication in Journal of Computational Electronics, 2003.
- [45] Christian Rivas, Roger Lake, William R. Frensley, Gerhard Klimeck, Phillip E. Thompson, Karl D. Hobart, Sean L. Rommel, and Paul R. Berger, "Full Band Modeling of the Excess Current in a Delta-Doped MBE Grown Silicon Tunnel Diode", accepted to Journal of Appl. Phys. (2003).

- [44] Fabiano Oyafuso, Gerhard Klimeck, Paul von Allmen, Tim Boykin, and R. Chris Bowen, "Strain Effects in large-scale atomistic quantum dot simulations", accepted for publication in physica status solidi b (2003).
- [43] Titus Sandu, Gerhard Klimeck, and Wiley Kirk, "Off-Center Electron Transport and Breakdown of Tsu-Esaki Formula in Resonant Tunneling Diodes due to Incoherent Scattering", Phys. Rev. B., Vol 68, 115320 (2002).
- [42] Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, Timothy B. Boykin, and Paul von Allmen, "Disorder Induced Broadening in Multimillion Atom Alloyed Quantum Dot Systems", Phys. Stat. Sol. (c), vol 0004, pg 1149-1152 (2003).
- [41] Gerhard Klimeck, Fabiano Oyafuso, R. Chris Bowen, Timothy B. Boykin, Thomas A. Cwik, Edith Huang, and Edward Vinyard, "3-D Atomistic Nanoelectronic Modeling on High Performance Clusters: Multimillion Atom Simulations", Superlattices and Microstructures, Vol. 31/2, pg 171-179, 2002.
- [40] Gerhard Klimeck, "Parallelization of the Nanoelectronic Modeling Tool (NEMO 1-D) on a Beowulf Cluster", Journal of Computational Electronics, Vol. 1, pp 75-79 (2002).
- [39] Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Atomistic Electronic Structure Calculations of Unstrained Alloyed Systems Consisting of a Million Atoms", Journal of Computational electronics, Vol. 1. Issue 3, pp. 317-321 (2002).
- [38] Seungwon Lee, Jeungnim Kim, Lars Jönsson, John W. Wilkins, Garnett Bryant, and Gerhard Klimeck, "Many-body levels of multiply charged and laser-excited InAs nanocrystals modeled by empirical tight binding", Phys. Rev. B 66, 235307 (2002).
- [37] Timothy B. Boykin, Gerhard Klimeck, R. Chris Bowen, and, Fabiano Oyafuso, "Diagonal parameter shifts due to nearest-neighbor displacements in empirical tight-binding theory", Phys. Rev. B 66, 125207 (2002).
- [36] Gerhard Klimeck, Fabiano Oyafuso, Timothy B. Boykin R. Chris Bowen, and, Paul von Allmen, "Development of a Nanoelectronic 3-D (NEMO 3-D) Simulator for Multimillion Atom Simulations and Its Application to Alloyed Quantum Dots (INVITED)", Computer Modeling in Engineering and Science (CMES) Volume 3, No. 5, pp 601-642 (2002).
- [35] Timothy B. Boykin, R. Chris Bowen, and, Gerhard Klimeck, "Electromagnetic coupling and gauge invariance in the empirical tight-binding method", Physical Review B, Vol. 63, pg. 245314 (2001).
- [34] Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Strong wavevector dependence of hole transport in heterostructures", Superlattices and Microstructures, Vol. 29, No. 3, pg. 187-216 (2001).
- [33] Seungwon Lee, Lars Jönsson, and John W. Wilkins, Garnett Bryant, and Gerhard Klimeck, "Electron-hole correlations in semiconductor quantum dots with tight-binding wave functions", Phys. Rev. B Vol. 63, 195318 (2001).
- [32] Gerhard Klimeck, "Indirect bandgap-like current flow in direct bandgap electron resonant tunneling diodes", Physica Status Solidi (b) Vol. 226, pg. 9-19 (2001)
- [31] Christian Rivas, Roger Lake, Gerhard Klimeck, William R. Frensley, Massimo V. Fischetti, Phillip E. Thompson, Sean L. Rommel, and Paul R. Berger, "Full Band Simulation of Indirect Phonon-Assisted Tunneling in a Silicon Tunnel Diode with Delta-Doped Contacts", Applied Physics Letters, Vol. 78, pg 814, (2001).
- [30] Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Off Zone Center (Indirect Bandgap Like) Hole Transport in Heterostructures", Phys. Rev. B., Vol. 63, pg. 195310 (2001).

- [29] Gerhard Klimeck, R. Chris Bowen, Timothy B. Boykin, and Thomas A. Cwik, "sp3s\* Tight-Binding Parameters for Transport Simulations in Compound Semiconductors", Superlattices and Microstructures Vol. 27, pp. 519-524 (2000).
- [28] Gerhard Klimeck, R. Chris Bowen, Timothy B. Boykin, Carlos Salazar-Lazaro, Thomas A. Cwik, and Adrian Stoica, "Si tight-binding parameters from genetic algorithm fitting", Superlattices and Microstructures, Vol. 27, No. 2/3, Mar 2000, pp. 77-88.
- [27] Timothy B. Boykin, R. Chris Bowen, Gerhard Klimeck, and Kevin L. Lear, "Resonant-tunneling diodes with emitter prewells", Appl. Phys. Lett, Vol. 75, 1302 (1999).
- [26] Timothy B. Boykin, Lisa J. Gamble, Gerhard Klimeck, and R. Chris Bowen, "Valence-band warping in tight-binding models", Phys. Rev. B Vol. 59, 7301 (1999).
- [25] Timothy B. Boykin, Roger K. Lake, Gerhard Klimeck, and Mukund Swaminathan, "Interface effects in tunneling models with identical real and complex dispersions", Phys. Rev. B Vol. 59, 7316 (1999).

# JOURNAL PUBLICATIONS (WORK PERFORMED PRIOR TO JPL)

- [24] Gerhard Klimeck, Dan Blanks, Roger Lake, R. Chris Bowen, Chenjing L. Fernando, Manhua Leng, William R. Frensley, Dejan Jovanovic, and Paul Sotirelis, "Writing Research Software in a Large Group for the NEMO Project", VLSI Design Vol. 8, pg 79 (1998).
- [23] Seal L. Rommel, Thomas E. Dillon, M. W. Dashiell, H. Feng, J. Kolodzey, Paul R. Berger, Phillip E. Thompson, Karl D. Hobart, Roger Lake, Alan C. Seabaugh, Gerhard Klimeck and Daniel K. Blanks, "Room temperature operation of epitaxially grown Si/Si\_0.5Ge\_0.5/Si resonant interband tunneling diodes", Applied Physics Letters, Vol. 73, 2191 (1998).
- [22] Gerhard Klimeck, Roger Lake and Daniel K. Blanks, "Numerical Approximations to the Treatment of Interface Roughness Scattering in Resonant Tunneling Diodes", Semicond. Sci. Technology Vol. 13, pg. A165 (1998).
- [21] Roger Lake, Gerhard Klimeck and Daniel K. Blanks, "Interface Roughness and Polar Optical Phonon Scattering in InGaAs/AlAs/InAs RTDs", Semicond. Sci. Technology Vol. 13, pg. A163 (1998).
- [20] Gerhard Klimeck, Roger. K. Lake, R. Chris Bowen, Chenjing L. Fernando and William R. Frensley, "Resolution of Resonances in a General Purpose Quantum Device Simulator", VLSI Design Vol. 6, pg. 107 (1998).
- [19] Roger. K. Lake, Gerhard Klimeck, R. Chris Bowen, Dejan Jovanovic, Paul Sotirelis and William R. Frensley, "A Generalized Tunneling Formula for Quantum Device Modeling", VLSI Design, Vol. 5, pg 9 (1998).
- [18] Gerhard Klimeck, Roger Lake and Daniel K. Blanks, "Role of interface roughness scattering in self-consistent resonant tunneling diode simulation", Phys. Rev. B, Vol. 58, 7279 (1998).
- [17] Timothy B. Boykin, Gerhard Klimeck, R. Chris Bowen, and Roger Lake, "Effective Mass Reproducibility of the Nearest-Neighbor sp<sup>3</sup>s\* Models: Analytic Results", Phys. Rev. B Vol. 56, 4102 (1997).
- [16] Gerhard Klimeck, Roger Lake, Dan Blanks, Chenjing L. Fernando, R. Chris Bowen, Ted Moise, and Y. C. Kao, "The Effects of Electron Screening Length and Emitter Quasi-Bound States on the Polar-Optical Phonon Scattering in Resonant Tunneling Diodes", Physica Status Solidi (b), Vol. 204, 408 (1997).
- [15] Roger Lake, Gerhard Klimeck, R. Chris Bowen, Dejan Jovanovic, Dan Blanks, Mukund Swaminathan, "Quantum Transport with Band-Structure and Schottky Contacts", Physica Status Solidi (b), Vol. 204, 354 (1997).

- [14] Roger Lake, Gerhard Klimeck, R. Chris Bowen and Dejan Jovanovic, "Single and multiband modeling of quantum electron transport through layered semiconductor devices", J. of Appl. Phys. 81, 7845 (1997).
- [13] R. Chris Bowen, Gerhard Klimeck, Roger Lake, William R. Frensley and Ted Moise, "Quantitative Resonant Tunneling Diode Simulation", J. of Appl. Phys. 81, 3207 (1997).
- [12] Roger K. Lake, Gerhard Klimeck, R. Chris Bowen, Chenjing L. Fernando, Manhua Leng, Ted Moise and Y. C. Kao, "Interface Roughness and Polar Optical Phonon Scattering And the Valley Current in Resonant Tunneling Devices", Superlattices and Microstructures, Vol. 20, p.279 (1996).
- [11] Jim A Tatum, Duncan L. MacFarlane, R. Chris Bowen, Gerhard Klimeck and William R. Frensley, "Ultrafast Characteristics of InGaP/InGaAlP Laser Amplifiers", IEEE J. of Quantum Electronics, Vol. 32, p.664 (1996).
- [10] Gerhard Klimeck, Roger K. Lake, R. Chris Bowen, William R. Frensley and Ted Moise, "Quantum Device Simulation with a Generalized Tunneling Formula", Appl. Phys. Lett., Vol. 67, p.2539 (1995).
- [9] R. Chris Bowen, William R. Frensley, Gerhard Klimeck, Roger K. Lake, "Transmission resonances and zeros in multi-band models", Phys. Rev. B., Vol. 52, p.2754 (1995)
- [8] Gerhard Klimeck, Roger Lake, Supriyo Datta, and Garnett Bryant, "Elastic and Inelastic Scattering in Quantum Dots in the Coulomb Blockade Regime", Phys. Rev. B, Vol. 50, 5484 (1994).
- [7] Guanlong Chen, Gerhard Klimeck, Supriyo Datta, G. H. Chen and W. A. Goddard III, "Resonant Tunneling through Quantum Dot Arrays", Phys. Rev. B, Vol. 50, p.8035 (1994).
- [6] Gerhard Klimeck, Guanlong L. Chen and Supriyo Datta, "Conductance Spectroscopy in Coupled Quantum Dots", Phys. Rev. B, Phys. Rev. B, Vol. 50, p.2316 (1994)
- [5] Roger Lake, Gerhard Klimeck, M. P. Anantram, and Supriyo Datta, "Rate Equations for the Phonon Peak in Resonant Tunneling Structures", Phys. Rev. B., Vol. 48, p.15132 (1993).
- [4] Roger Lake, Gerhard Klimeck, and Supriyo Datta, "Rate Equations from the Keldysh Formalism Applied to the Phonon Peak in Resonant-Tunneling Diodes", Phys. Rev. B, Vol. 47, p.6427 (1993).
- [3] Yong Lee, Michael J. McLennan, Gerhard Klimeck, Roger Lake and Supriyo Datta, "Quantum Kinetic Analysis of Mesoscopic Systems: Linear Response", Superlattices and Microstructures, Vol. 11, p.137 (1992).
- [2] Gerhard Klimeck, D. S. Elliott and M. W. Hamilton, "Laser-Bandwidth-Induced Fluctuations in the Intensity Transmitted by a Fabry-Perot Interferometer", Phys. Rev. A, Vol. 44, p.3222 (1991).
- [1] Cheng Xie, Gerhard Klimeck and D. S. Elliott, "Generation and Intensity Correlation Measurements of the Real Gaussian Field", Phys. Rev. A Vol. 41, p.6376 (1990).

# PEER REVIEWED CONFERENCE PROCEEDINGS (WORK PERFORMED AT JPL)

These peer-reviewed proceedings articles are typically extended abstracts made available to conference participants. Some of the articles are also publicly available in conference archives such as IEEE IEDM, IEEE DRC, IEEE SISPAD, IEEE AP-S, and Inst. Phys. Conf. Ser.

The conference participation is also shown in the list of conferences.

- [P46] Paul von Allmen, Seungwon Lee, Fabiano Oyafuso, Gerhard Klimeck, and Olga Lazarenkova, "Coupled electron and nuclear spin dynamics in InAs quantum dots: impact on single and two-qubit operations", Quantum Dot 2004, Banff, Alberta, Canada, May 10-13, 2004.
- [P45] Seungwon Lee, Olga Lazarenkova, Fabiano Oyafuso, Paul von Allmen, and Gerhard Klimeck, "Effect of Wetting Layers on Strain and Electronic Structures of Self-Assembled Quantum Dots", Quantum Dot 2004, Banff, Alberta, Canada, May 10-13, 2004.
- [P44] Olga L. Lazarenkova, Paul von Allmen, Seungwon Lee, Fabiano Oyafuso, and Gerhard Klimeck, "Atomistic-Level Simulation of the Vibration Spectrum of Quantum Dot Crystals", Quantum Dot 2004, Banff, Alberta, Canada, May 10-13, 2004.
- [P43] Mark Kordon, Gerhard Klimeck, Dave Hanks, Hook Hua, "Evolutionary Computing for the Design Search and Optimization of Space Vehicle Power Subsystems", accepted in proceedings of IEEE Aerospace Conference, Bug Sky, Montana, March 2004.
- [P42] Seungwon Lee, Paul von Allmen, Fabiano Oyafuso, Gerhard Klimeck, and K. B. Whaley, "Electron spin dephasing and decoherence by interaction with nuclear spins in self-assembled quantum dots", accepted in proceedings of Winter International Symposium on Information and Communication Technologies, January 5-8, 2004, Cancun, Mexico.
- [P41] Gerhard Klimeck, Timothy B. Boykin, Mark Eriksson, Mark Friesen, S. N. Coppersmith, Paul von Allmen, Fabiano Oyafuso, and Seungwon Lee, "Conduction band valley splitting in silicon nano-structures", Sixth International Conference on New Phenomena in Mesoscopic Structures, Fourth International Conference on Surfaces and Interfaces of Mesoscopic Devices, December 1-5, 2003, Maui, Hawaii.
- [P40] Seungwon Lee, Fabiano Oyafuso, Paul von Allmen, and Gerhard Klimeck, "Numerical surface treatment for finite-extent semiconductor nanostructures", 14th Workshop on Modelling and Simulation of Electron Devices, Barcelona, Spain, October 16-17 2003, pages 171-174.
- [P39] Hans Kosina, Gerhard Klimeck, Michail Nedjalkov, Siegfried Selberherr, "Comparison of Numerical Quantum Device Models", International Conference on Simulation of Semiconductor Processes and Devices (SISPAD 2003), September 3-5, 2003, Boston, MA.
- [P38] Gerhard Klimeck, Gary Yagi, Robert Deen, Myche McAuley, Eric DeJong, Fabiano Oyafuso "Near Real-Time Parallel Image Processing using Cluster Computers", International Conference on Space Mission Challenges for Information Technology (SMC-IT), Pasadena, CA July 13-16, 2003
- [P37] Fabiano Oyafuso, Gerhard Klimeck, Timothy B. Boykin, R. Chris Bowen, and Paul von Allmen, "Study of Strain Boundary Conditions and GaAs Buffer Sizes in InGaAs Quantum Dots", Extended Abstract in Proceedings of International Workshop on Computational Electronics, Frascati, Rome, Italy, May 25-28, 2003.
- [P36] Gerhard Klimeck, Phillip Stout and R. Chris Bowen, "Quantum and semi-classical transport in RTDs using NEMO 1-D", Extended Abstract in Proceedings of International Workshop on Computational Electronics, Frascati, Rome, Italy, May 25-28, 2003.
- [P35] Jeremy Green, Corrie Farmer, Michel Garcia, Hock Koon Lee, Colin Stanley, Charles Ironside, Gerhard Klimeck, and Roger Lake, "Quantum cascade laser simulation using sp3s\* full Brillouin zone tight-binding model", Accepted in Proceedings of CLEO/Europe 2003, Munich 22-27 June 2003.
- [P34] Gerhard Klimeck, Fabiano Oyafuso, Timothy B. Boykin, R. Chris Bowen, Paul von Allmen, "Study of Alloy Disorder in Quantum Dots through Multi-million Atom Simulations", Proceedings of Nanotech2003 (including MSM 2003 and ICCN 2003), February 23-27, 2003, San Francisco.

- [P33] Gerhard Klimeck, Fabiano Oyafuso, Timothy B. Boykin, R. Chris Bowen, Paul von Allmen, "Status of the Nanoelectronic Modeling tool (NEMO 1-D and 3-D) and its planned extension to Spintronics", The first International Workshop on Quantum Dots for Quantum Computing and Classical Size Effect Circuits (IWQDQC), Kochi, Japan, Jan 26-28, 2002
- [P32] Tom Cwik, Gerhard Klimeck, Myche McAuley, Bob Deen and Eric Dejong, "Applications on High Performance Cluster Computers Production of Mars Panoramic Mosaic Images", Proceedings of the 2001 AMOS Technical Conference, September 10-14, 2001, Maui.
- [P31] Gerhard Klimeck "Full Brillouin-Zone, Charge Self-consistent Quantum Transport Simulation Enabled by Parallelization of the Nanoelectronic Modeling Tool (NEMO 1-D) on a Beowulf Cluster", 8th International Workshop on Computational Electronics, October 15-18, 2001, Univ. of Illinois, Urbana Champaign.
- [P30] Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Atomistic Electronic Structure Calculations of Unstrained Alloyed Systems Consisting of a Million Atoms", 8th International Workshop on Computational Electronics, October 15-18, 2001, Univ. of Illinois, Urbana Champaign.
- [P29] Tom Cwik, Gerhard Klimeck, Charles Norton, Thomas Sterling, Frank Villegas and Ping Wang, "The Use of Cluster Computers Systems for NASA/JPL Applications", Proceedings of AIAA Space 2001 Conference and Exposition Albuquerque, New Mexico 28-30, Aug. 2001.
- [P28] Tom Cwik, Gerhard Klimeck, and Frank Villegas, "Large-Scale Design and Optimization Using Cluster Computers", IEEE AP-S International Symposium and USNC/URSI National Radio Science Symposium", Boston, MA, July 8-13 (2001).
- [P27] Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Atomistic simulation of quantum dots including strain and bandstructure and full band simulation of hole transport in 1-D heterostructures", 7th International Workshop on Computational Electronics. Book of Abstract. IWCE, pp 6-7, (2000)
- [P26] Didier Keymeulen, Gerhard Klimeck, R. Zebulum, Adrian Stoica, Yili Jin, Carlos-Salazar Lazaro, "EHWPack: an Evolvable Hardware Environment using the Spice Simulator and the Field Programmable Transistor Array", In the Proceedings of ANNIE12000 (Smart Engineering System Design), St. Louis, MO, November 5-8, 2000
- [P25] Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Transverse Momentum Dependence of Electron and Hole Tunneling in a Full Band Tight-Binding Simulation", Proceedings of the 27th international Symposium on Compound Semiconductors (ISCS), IEEE, (2000)
- [P24] Adrian Stoica, Didier Keymeulen, Ricardo Zebulum, Anil Thakoor, Taher Daud, Gerhard Klimeck, Yili Jin, R. Tawel, Vu Duong, "Evolution of analog circuits on field programmable transistor arrays", Proceedings of 2<sup>nd</sup> NASA/DoD Workshop on Evolvable Hardware, July 13-15, pg. 99-108, 2000.
- [P23] Didier Keymeulen, Gerhard Klimeck, Ricardo Zebulum, Adrian Stoica, and Carlos Salazar-Lazaro, "EHWPack: A Parallel Software/Hardware Environment for Evolvable Hardware", In Whitley Darrell (eds.), Proceedings of the Genetic and Evolutionary Computation Conference (GECCO-2000), July 8-12, 2000, Las Vegas, Nevada USA. San Francisco, CA: Morgan Kaufmann.
- [P22] Adrian Stoica, Gerhard Klimeck, Carlos Salazar-Lazaro, Didier Keymeulen, and Anil Thakoor, "Evolutionary Design of Electronic Devices and Circuits", Proceedings of the 1999 Congress on Evolutionary Computation, IEEE, CEC 99, Vol. 2, Pages: 1271-1278.
- [P21] Tom Cwik and Gerhard Klimeck, "Genetically Engineered Microelectronic Infrared Filters", Proceedings of the First NASA/DoD Workshop on Evolvable Hardware, IEEE 1999, Page(s): 242-246.

- [P20] Gerhard Klimeck, Carlos H. Salazar-Lazaro, Adrian Stoica, and Thomas Cwik, "Genetically Engineered Nanoelectronics", Proceedings of the First NASA/DoD Workshop on Evolvable Hardware, IEEE 1999, Page(s): 247 -248.
- [P19] Tom Cwik and Gerhard Klimeck, "Integrated Design and Optimization of Microelectronic Devices", Proceedings of 1999 Aerospace Conference, IEEE Volume: 5, 1999, Page(s): 131 -138.
- [P18] Gerhard Klimeck, Carlos H. Salazar-Lazaro, Adrian Stoica, and Tom Cwik, "Genetically Engineered" Nanostructure Devices, in "Materials in Space Science, Technology, and Exploration", MRS Symposium Proceedings, Vol. 551, pg. 149 (1999).

## CONFERENCE PROCEEDINGS (WORK PERFORMED PRIOR TO JPL)

- [P17] Daniel K. Blanks, Gerhard Klimeck, Roger Lake, R. Chris Bowen, Manhua Leng, Chenjing Fernando, William R. Frensley, and Dejan Jovanovic, "NEMO Quantum Device Simulator", 1998 Government Microcircuit Applications Conference Digest of Papers (GOMAC), March 1998, p. 218.
- [P16] R. Chris Bowen, Chenjing Fernando, Gerhard Klimeck, A. Chatterjee, Daniel Blanks, Roger Lake, J. Hu, J. Davis, M. Kularni, S. Hattangady, and I.C. Chen, "Physical Oxide Extraction and Versification using Quantum Mechanical Simulation", Proceedings of IEDM 1997, IEEE, 869 (1997).
- [P15] R. Chris Bowen, Chenjing L. Fernando, Gerhard Klimeck, Amitava Chatterjee, Dan Blanks, Roger Lake, Jerry Hu, Joseph Davis, Mak Kulkarni, Sunil Hattangady, and Ih-Chin Chen, "Dopant Fluctuations and Quantum Effects in Sub-0.1um CMOS", Proceedings of the 1997 International Semiconductor Device Research Symposium, p. 1.
- [P14] Roger Lake, Berinder Brar, Glen Wilk, Alan Seabaugh, and Gerhard Klimeck, "Resonant Tunneling in Disordered Materials such as SiO2/Si/SiO2", Proceedings of the 24th International Symposium on Compound Semiconductors, September 8-11, San Diego, CA, (1997). Inst. Phys. Conf. Ser. 156: 617-620, 1998.
- [P13] Daniel K. Blanks, Gerhard Klimeck, Roger Lake, Dejan Jovanovic, R. Chris Bowen, Chenjing Fernando, William R. Frensley, and Manhua Leng, "NEMO: General Release of a New Comprehensive Quantum Device Simulator", Proceedings of the 24th International Symposium on Compound Semiconductors, IEEE, NJ (1997). Inst. Phys. Conf. Ser. 156: 639-642, 1998.
- [P12] J. P. A. van der Wagt, Alan Seabaugh, Gerhard Klimeck, Ed A. Beam III, Timothy, B. Boykin, R. Chris Bowen, and Roger Lake, "Ultralow Current Density RTDs for Tunneling-based SRAM", Proceedings of the 24th International Symposium on Compound Semiconductors, September 8-11, San Diego, CA, (1997). Inst. Phys. Conf. Ser. 156: 601-604, 1998.
- [P11] Dan Blanks, Gerhard Klimeck, Roger Lake, R. Chris Bowen, William R. Frensley, Manhua Leng, and Chenjing L. Fernando, "Nanoelectronic Modeling (NEMO): A New Quantum device Simulator", Proceedings of The Second NASA Device Modeling Workshop, August 7-8, 1997, page 70-84, Edited by Subhash Saini. You can request a copy of this from NAS Library, MS 258-5, NASA Ames research center, Moffett Field, CA 94035-1000.
- [P10] Gerhard Klimeck, Timothy B. Boykin, R. Chris Bowen, Roger Lake, Dan Blanks, Ted Moise, Y. C. Kao, and William R. Frensley, "Quantitative Simulation of Strained InP-Based Resonant Tunneling Diodes", in Proceedings of the 1997 55<sup>th</sup> IEEE Device Research Conference Digest, IEEE, NJ, p. 92 (1997).
- [P9] Gerhard Klimeck, Dan Blanks, Chris Bowen, Bobby Brar, Tom Broekaert, Gary Frazier, Dejan Jovanovic, Roger Lake, Ted Moise, Alan Seabaugh, Glen Wilk, and Paul van der Wagt, "Design and Implementation of Resonant Tunneling Devices into Circuits and Applications", in Proceedings of PHASDOM97, Phantoms Strategic Domain Meetings, Aachen, Germany, March 10-13, 1997.

- [P8] Roger Lake, Gerhard Klimeck, "Experimentally Verified Quantum Device Simulations Based on Multiband Models, Hartree Self-consistency, and Scattering Assisted Charging", in Proceedings of the 1996 54th IEEE Device Research Conference Digest, IEEE, NJ, p. 174, 1996
- [P7] William R. Frensley, R. Chris Bowen, Chenjing Fernando, Gerhard Klimeck, and Roger Lake, "Quantitatively Accurate Simulation of Quantum Semiconductor Devices", Proceedings of International Workshop on Physics and Computer Modeling of Devices Based on Low-Dimensional Structures. IEEE Comp. Soc. Press, Los Alamitos, CA, p.2, 1996.
- [P6] Gerhard Klimeck, Roger Lake, Chenjing L. Fernando, R. Chris Bowen, Dan Blanks, Manhua Leng, Ted Moise, Y. C. Kao, and William R. Frensley in "Quantum Devices and Circuits" edited by K. Ismail, S. Bandyopadhyay, ad J. P. Leburton, Imperial Press London (1996).
- [P5] Gerhard Klimeck, Roger Lake, R. Chris Bowen, William R. Frensley and Daniel Blanks, "Nanoelectronic Modeling (NEMO)", in Proceedings of the 1995 53rd Device Research Conference Digest, IEEE, NJ p. 52, 1995.
- [P4] R. Chris Bowen, William R. Frensley and Gerhard Klimeck, "Efficient I-V simulation of quantum devices using full bandstructure models", Proceeding of IEEE Cornell Conference on Advanced Concepts in High Speed Semiconductor Devices and Circuits, IEEE, New York, NY, p.435, 1995.
- [P3] Supriyo Datta, Gerhard Klimeck, Roger K. Lake and M. P. Anantram, "Resonant Tunneling devices: Effect of Scattering", International Symposium on Compound Semiconductors, San Diego, Sept. 18-24, 1994. Inst. Phys. Conf. Ser. No 141; Chapter 7, p.775, (1995)
- [P2] Gerhard Klimeck, Roger K. Lake, and Supriyo Datta, "The Phonon Peak in Resonant Tunneling Diodes", Journal of the Electrochemical Society, (1995).
- [P1] Gerhard Klimeck, Roger Lake, Supriyo Datta, and Garnett Bryant, "High Bias Transport through Quantum Dots", Journal of the Electrochemical Society, (1995).

## **INVITED CONFERENCES**

- [I41] Gerhard Klimeck and Mark Lundstrom, "The Network for Computational Nanotechnology", National Nanotechnology Initiative: From Vision to Commercialization, Keynote Address, Washington DC, March 31-April 2, 2004.
- [I40] Mark Lundstrom and Gerhard Klimeck, "The Network for Computational Nanotechnology", Nanotech 2004, Keynote Address, Boston, MA, March 8-11, 2004.
- [I39] Mark Lundstrom and Gerhard Klimeck, "Network for Computational Nanotechnology", Supercomputing Conference 2003, Birds of a Feather Session on HPC Innovation for Nanotechnology, Phoenix, AZ, November 16-21, 2003.
- [I38] Mark Lundstrom and Gerhard Klimeck"Device Simulation at the Molecular Scale", Silicon Nanoelectronics and Beyond Workshop, Panel Session IV Tools and Methodologies for Nanoelectronic Design, Hillsboro, OR, October 29-30, 2003, sponsored by NSF, SRC, Intel.
- [I37] Gerhard Klimeck, Fabiano Oyafuso, Seungwon Lee, Timothy B. Boykin, Paul von Allmen, R. Chris Bowen, and Olga Lazarenkova. "Development of the Nanoelectronic Modeling tool (NEMO-3D) for multimillion atom quantum dots", Computational Approaches Toward the Electronic Properties of Quantum Dots Workshop, Chicago, September 22-24, 2003, sponsored by DARPA.
- [I36] Gerhard Klimeck, Fabiano Oyafuso, Paul von Allmen, Timothy B. Boykin, and R. Chris Bowen, "Study of Alloy Disorder in Quantum Dots through Multi-million Atom Simulations", CERION II Workshop Bilbao (Spain) September 2-6, 2003.

- [I35] Gerhard Klimeck, Timothy B. Boykin, Mark Eriksson, Mark Friesen, Susan Coppersmith, Fabiano Oyafuso, Paul von Allmen, Seungwon Lee, and K. Birgitta Whaley, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", NSA / ARDA / ARO Quantum Computing Technology Workshop, Nashville, TN, August 18-22, 2003.
- [I34] Gerhard Klimeck, Roger Lake, R. Chris Bowen, Tim Boykin, Dan Blanks, William R. Frensley, Fabiano Oyafuso, Seungwon Lee, Paul von Allmen, Olga Lazarenkova, Thomas A. Cwik, "Key elements in NEMO to quantitative nano-scale carrier transport analysis in semiconductors", Workshop on molecular conduction, Purdue University, July 8-11, 2003.
- [I33] Paul von Allmen, Seungwon Lee, Fabiano Oyafuso, Gerhard Klimeck, Tim Boykin, "Empirical Atomic Level Simulations for QC Applications", THINQC, June 9-10, 2003, Harpers Ferry.
- [I32] Gerhard Klimeck, Gary Yagi, Robert Deen, Myche McAuley, Eric DeJong, and Fabiano Oyafuso, "Near Real-Time Parallel Image Processing using Cluster Computers", Quality Mission Software Workshop, May 13-15, 2003, Rehoboth Beach, Delaware.
- [I31] Gerhard Klimeck, Fabiano Oyafuso, Paul von Allmen, Timothy B. Boykin, and R. Chris Bowen, "Study of Alloy Disorder in Quantum Dots through Multi-million Atom Simulations", Nanotech2003 (including MSM 2003 and ICCN 2003), February 23-27, 2003, San Francisco.
- [I30] Gerhard Klimeck, Fabiano Oyafuso, Timothy B. Boykin, R. Chris Bowen, and Paul von Allmen, "Development of a 3-D tight binding-based electronic structure simulator for multi-million atom systems (NEMO 3-D)", Advanced Heterostructure Workshop, Hapuna Beach, HI, Dec. 1-6, 2002.
- [I29] Gerhard Klimeck, Fabiano Oyafuso, Paul von Allmen, Timothy B. Boykin, and R. Chris Bowen, "Nanoelectronic Modeling: NEMO 1-D: Design, Optimization, Synthesis, NEMO 3-D: Fundamental Limits", Nanoelectronics Planet Fall 2002, Conference and Expo, NY, NY, Nov. 18-19, 2002.
- [I28] Paul von Allmen and Gerhard Klimeck, "Transport Simulation of Precessing Spin Distribution across Semiconductor Heterojunctions", DARPA Spintronics Workshop, Delray Beach, FL, Sep 30 Oct 4, 2002.
- [I27] Gerhard Klimeck, Fabiano Oyafuso, Timothy B. Boykin, and Paul von Allmen, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", NSA / ARDA / ARO Quantum Computing Technology Workshop, Nashville, TN, August 19-23, 2002.
- [I26] Gerhard Klimeck, Fabiano Oyafuso, Timothy B. Boykin, R. Chris Bowen, and Paul von Allmen, "NEMO 3-D: Electronic Structure Simulations Including over Ten Million Atoms", Nanospace 2002, Galveston, TX, June 24-28, 2002
- [I25] Gerhard Klimeck, Fabiano Oyafuso, Timothy B. Boykin, R. Chris Bowen, Paul von Allmen, "Status of the Nanoelectronic Modeling tool (NEMO 1-D and 3-D) and its planned extension to Spintronics", The first International Workshop on Quantum Dots for Quantum Computing and Classical Size Effect Circuits (IWQDQC), Kochi, Japan, Jan 26-28, 2002
- [I24] Nikzad Toomarian, Amir Fijani, Gerhard Klimeck, Rosa Leon, Yuming Qiu, "Quantum Dots Based Rad-Hard Computing and Sensors", Keynote, CMP Cientifica, TNT 2001 Conference, Sept 3-7, 2001.
- [I23] Gerhard Klimeck, "Applications of quantum transport in devices", Advanced Research Workshop on Quantum Transport in Semiconductors, Maratea, Italy, June 17-22 (2001).
- [I22] Gerhard Klimeck, "Nanoelectronic Modeling (NEMO): Moving from commercial grade 1-D simulation to prototype 3-D simulation", March Meeting of American Physical Society, March 12-16, Seattle, WA (2001).

- [I21] Gerhard Klimeck, R. Chris Bowen, Timothy B. Boykin, "Atomistic 3-D Simulation of Nanoelectronic Structures", 2nd Workshop on Computational Materials and Electronics, Motorola University, Tempe, Arizona, Nov 9-10, (2000).
- [I20] Gerhard Klimeck, R. Chris Bowen, Thomas A. Cwik, and Timothy B. Boykin, "Development of a 3-D Nanoelectronic Device Modeling Tool (NEMO 3-D)", DARPA Workshop on Gigascale Integration, Washington DC, May 5, 2000.
- [I19] Gerhard Klimeck, R. Chris Bowen, Timothy B. Boykin, Carlos Salazar-Lazaro, Thomas A. Cwik, and Adrian Stoica, "Simulator Development for Nanoelectronic Device", 3rd NASA Workshop on Device Modeling, NASA Ames Research Center, August 26-29, 1999.
- [I18] Gerhard Klimeck, Chris Bowen, Tim Boykin, Fabiano Oyafuso, Carlos Salazar-Lazaro, Adrian Stoica, and Tom Cwik, "Nanoelectronic Modeling at JPL", DARPA Ultra Electronics Program Review, Oct 18-21, 1998, Estes Park, CO.
- [I17] Gerhard Klimeck, Chris Bowen, Tim Boykin, Fabiano Oyafuso, Tom Cwik, Carlos Salazar-Lazaro, and Adrian Stoica, "The Nanoelectronic Modeling Tool NEMO and its extension to High Performance Computing", ICSDT 98 6th International Conference on Simulation of Devices and Technologies, Cape Town, South Africa, Oct 14-16, 1998.
- [I16] Gerhard Klimeck, Carlos H. Salazar-Lazaro, Adrian Stoica, and Tom Cwik, "Structural Analysis Using Quantum Mechanical Electron Transport Simulations Driven by a Genetic Algorithm", Second Workshop on Characterization, Future Opportunities and Applications of 6.1Å III-V Semiconductors, Organized by ONR, NRL, and DARPA, August 24-26, 1998 Naval Research Laboratory, Washington, DC.

# INVITED CONFERENCES (WORK PERFORMED PRIOR TO JPL)

- [I15] Gerhard Klimeck, Daniel K. Blanks, Roger Lake, "NEMO: A Novel 1-D Quantum Device Simulator", DARPA/Rome Lab Composite CAD Program Principal Investigator Meeting, Huntsville, AL, December 1-3, 1997
- [I14] Gerhard Klimeck, Roger Lake, Daniel K. Blanks, "NEMO: Quantitative Resonant Tunneling Diode Simulation", 1997 DARPA ULTRA Electronics and Advanced Microelectronics Program Review, October 26-31, Santa Fe, NM (1998).
- [I13] R. Chris Bowen, Chenjing L. Fernando, Gerhard Klimeck, Amitava Chatterjee, Dan Blanks, Roger Lake, Jerry Hu, Joseph Davis, Mak Kulkarni, Sunil Hattangady, and Ih-Chin Chen, "Dopant Fluctuations and Quantum Effects in Sub-0.1um CMOS", 1997 International Semiconductor Device Research Symposium, Virginia, Dec. 1997.
- [I12] Gerhard Klimeck, Dan Blanks, Roger Lake, R. Chris Bowen, William R. Frensley, Manhua Leng, and Chenjing Fernando, "Nanoelectronic Modeling (NEMO): A New Quantum Device Simulator", The Second NASA Device Modeling Workshop, Aug. 7-8 1997, NASA Ames Research Center, Moffett Field, CA.
- [I11] Gerhard Klimeck, Roger Lake, R. Chris Bowen, Dan Blanks, Manhua Leng, Chenjing Fernando, William R. Frensley, Dejan Jovanovic, Paul Sotirelis, "The NEMO Project or Writing Software in a Large Research Group", International Workshop on Computational Electronics, South Bend, IN, May 1997.
- [I10] Gerhard Klimeck, Dan Blanks, Chris Bowen, Bobby Brar, Tom Broekaert, Gary Frazier, Dejan Jovanovic, Roger Lake, Ted Moise, Alan Seabaugh, Glen Wilk, and Paul van der Wagt, "Design and Implementation of Resonant Tunneling Devices into Circuits and Applications", PHASDOM97, Phantoms Strategic Domain Meeting, Aachen, Germany, March 10-13, 1997.

- [19] William R. Frensley, R. Chris Bowen, Chenjing L. Fernando, Gerhard Klimeck, Manhua Leng, Dan Blanks and Ted Moise, "Resonant Tunneling as a Probe of Electron Transport in Semiconductor Heterostructures", First International Conference on Open Problems in Charged Particle Transport, Paris, France, June 1996.
- [I8] Roger Lake, Gerhard Klimeck, R. Chris Bowen, Chenjing L. Fernando, Ted Moise, Daniela Francovicchio, and Y. C. Kao, "Transport Physics of Tunnel Devices", Third International Symposium on Nanostructures and Mesoscopic Structures, Santa Fe, NM, May 19-24, 1996.
- [17] Roger Lake, Gerhard Klimeck, Chenjing L. Fernando, R. Chris Bowen, Ted Moise, Y. C. Kao, and Daniela Francovicchio, "Interface Roughness and Polar Optical Phonon Scattering in RTDs: theory, modeling and experiment", 23rd Conference on the Physics and Chemistry of Semiconductor Interfaces, La Jolla, CA, Jan. 21-25, 1996.
- [I6] William R. Frensley, R. Chris Bowen, Chenjing L. Fernando, Gerhard Klimeck, Roger Lake and Dan Blanks, "Quantitative Accurate Simulation of Quantum Semiconductor Devices", Workshop on Physics and Computer Modeling of Devices Based on Low Dimensional Structures, University of Aizu, Aizu-Wakamatsu, Japan, Nov. 1995.
- [15] William R. Frensley, James R. Hellums, Chenjing L. Fernando, R. Chris Bowen, and Gerhard Klimeck, "Open System Boundary Conditions for the Time-Dependent and Steady State Schrödinger Equations", Workshop on Density Matrix Methods at the Institute for Theoretical Atomic and Molecular Physics, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, Aug. 1995.
- [I4] William R. Frensley, Chenjing L. Fernando, R. Chris Bowen, and Gerhard Klimeck, "Modeling Tools for the Development of Quantum and Conventional Semiconductor Heterostructure Devices", Government Microcircuit Applications Conference (GOMAC), San Diego, CA, Nov. 1994.
- [I3] Supriyo Datta, Gerhard Klimeck, Roger Lake, Yong Lee and Michael J. McLennan, "Quantum Device Simulation Including Interactions", International Workshop on Computational Electronics, Portland, May 18-20 1994.
- [I2] Supriyo Datta, Gerhard Klimeck, and Roger Lake, "Resonant tunneling diodes: Effects of Scattering on the Valley Current", International Symposium on Compound Semiconductors, San Diego, Sept. 18-24, 1994. Inst. Phys. Conf. Ser. 141: 770-775, 1995.
- [I1] Supriyo Datta, Roger Lake, and Gerhard Klimeck, "Quantum Device Simulation", Microwave Theory and Techniques Symposium, Workshop on Combined Self-Consistent Particle Transport Simulation and Full Wave Dynamic Field Simulation for Monolithic Solid State Device and Circuit Calculations, Atlanta, June 18, 1993.

## CONTRIBUTED CONFERENCES (WORK PERFORMED AT JPL)

- [C116] Paul von Allmen, Seungwon Lee, Fabiano Oyafuso, Gerhard Klimeck, and Olga Lazarenkova, "Coupled electron and nuclear spin dynamics in InAs quantum dots: impact on single and two-qubit operations", Quantum Dot 2004, Banff, Alberta, Canada, May 10-13, 2004.
- [C115] Seungwon Lee, Olga Lazarenkova, Fabiano Oyafuso, Paul von Allmen, and Gerhard Klimeck, "Effect of Wetting Layers on Strain and Electronic Structures of Self-Assembled Quantum Dots", Quantum Dot 2004, Banff, Alberta, Canada, May 10-13, 2004.
- [C114] Olga L. Lazarenkova, Paul von Allmen, Seungwon Lee, Fabiano Oyafuso, and Gerhard Klimeck, "Atomistic-Level Simulation of the Vibration Spectrum of Quantum Dot Crystals", Quantum Dot 2004, Banff, Alberta, Canada, May 10-13, 2004.
- [C113] Gerhard Klimeck, T. B. Boykin, M. Eriksson, M. Friesen, S. N. Coppersmith, P. von Allmen, F. Oyafuso, S. Lee, "Conduction band valley splitting in Si", March Meeting of the American Physical Society, March 22-26, Montreal, CA (2004).

- [C112] Seungwon Lee, Paul von Allmen, Fabiano Oyafuso, Gerhard Klimeck, K Birgitta Whaley, "Effect of electron-nuclear spin interactions on electron-spin qubits localized in self-assembled quantum dots", March Meeting of the American Physical Society, March 22-26, Montreal, CA (2004).
- [C111] Seungwon Lee, Fabiano Oyafuso, Paul von Allmen, Gerhard Klimeck, "Efficient boundary condition for the electronic structure of embedded semiconductor nanostructures", March Meeting of the American Physical Society, March 22-26, Montreal, CA (2004).
- [C110] Paul von Allmen, Seungwon Lee, Fabiano Oyafuso, Gerhard Klimeck, "Effect of nuclear spin dynamics on quantum computing operations in spin based qubits", March Meeting of the American Physical Society, March 22-26, Montreal, CA (2004).
- [C109] Paul von Allmen, Seungwon Lee, Fabiano Oyafuso, Gerhard Klimeck, "Sensitivity and response time of palladium nanowire hydrogen sensors", March Meeting of the American Physical Society, March 22-26, Montreal, CA (2004).
- [C108] Olga L. Lazarenkova, Paul von Allmen, Fabiano Oyafuso, Seungwon Lee, Gerhard Klimeck, "Effect of strain on the phonon dispersion in Ge/Si quantum dot superlattices with an atomistic level model", March Meeting of the American Physical Society, March 22-26, Montreal, CA (2004).
- [C107] Mark Kordon, Gerhard Klimeck, Dave Hanks, and Hook Hua, "Evolutionary Computing for the Design Search and Optimization of Space Vehicle Power Subsystems", IEEE Aerospace Conference, Big Sky, Montana, March 2004. Proceedings P43.
- [C106] Gerhard Klimeck, Paul von Allmen, Seungwon Lee, Fabiano Oyafuso, Olga Lazarenkova, Timothy B. Boykin, "Nanoelectronic Modeling (NEMO) for Realistic Simulations of Solid-State Quantum Computing Gates", DARPA Focused Quantum Systems (FoQuS) Workshop, Falls Church, VA, Jan 28-29 (2004).
- [C105] Richard J. Terrile, Chris Adami, Michael Ferguson, Wolfgang Fink, Terry Huntsberger, Gerhard Klimeck, Mark Kordon, Erick Mjolsness, Savio Chau, "Evolutionary Computing Technologies for Space Systems", JPL conference on internal research and development, December 4, 2003, Pasadena, CA.
- [C104] Gerhard Klimeck, Timothy B. Boykin, Mark Eriksson, Mark Friesen, S. N. Coppersmith, Paul von Allmen, Fabiano Oyafuso, and Seungwon Lee, "Conduction band valley splitting in silicon nano-structures", Sixth International Conference on New Phenomena in Mesoscopic Structures, Fourth International Conference on Surfaces and Interfaces of Mesoscopic Devices, December 1-5, 2003, Maui, Hawaii.
- [C103] Seungwon Lee, Fabiano Oyafuso, Paul von Allmen, and Gerhard Klimeck, "Numerical surface treatment for finite-extent semiconductor nanostructures", 14th Workshop on Modelling and Simulation of Electron Devices, Barcelona, Spain, October 16-17 2003.
- [C102] Gerhard Klimeck, Fabiano Oyafuso, Timothy B. Boykin, Paul von Allmen, Seungwon Lee, and Olga Lazarenkova, "Development of a 3-D Nanoelectronic Modeling Tool (NEMO 3-D)", accepted in 14th Workshop on Modelling and Simulation of Electron Devices, Barcelona (Casa Convalescència) 16, 17 October 2003.
- [C101] Hans Kosina, Gerhard Klimeck, Michail Nedjalkov, Siegfried Selberherr, "Comparison of Numerical Quantum Device Models", International Conference on Simulation of Semiconductor Processes and Devices (SISPAD 2003), September 3-5, 2003, Boston, MA.
- [C100] Seungwon Lee, Gerhard Klimeck, K. Birgitta Whaley, "Electron-spin g-factor engineering with SiGe heterostructures", Spintech II International Conference and School, Semiconductor Spintronics and Quantum Information Technology. August 4-8, 2003 Brugge, Belgium.

- [C99] Gerhard Klimeck, Gary Yagi, Robert Deen, Myche McAuley, Eric DeJong, Fabiano Oyafuso "Near Real-Time Parallel Image Processing using Cluster Computers", International Conference on Space Mission Challenges for Information Technology (SMC-IT), Pasadena, CA July 13-16, 2003.
- [C98] Fabiano Oyafuso, Gerhard Klimeck, Timothy B. Boykin, R. Chris Bowen, and Paul von Allmen, "Study of Strain Boundary Conditions and GaAs Buffer Sizes in InGaAs Quantum Dots", International Workshop on Computational Electronics, Frascati, Rome, Italy, May 25-28, 2003.
- [C97] Gerhard Klimeck, Phillip Stout and R. Chris Bowen, "Quantum and semi-classical transport in RTDs using NEMO 1-D", International Workshop on Computational Electronics, Frascati, Rome, Italy, May 25-28, 2003.
- [C96] Jeremy Green, Corrie Farmer, Michel Garcia, Hock Koon Lee, Colin Stanley, Charles Ironside, Gerhard Klimeck, and Roger Lake, "Quantum cascade laser simulation using sp3s\* full Brillouin zone tight-binding model", CLEO/Europe 2003, Munich 22-27 June 2003.
- [C95] Titus Sandu, Gerhard Klimeck, and Wiley P. Kirk, "Structure of Transverse Electron Current in Resonant Tunneling Diodes and Breakdown of Tsu-Esaki Formula", March Meeting of American Physical Society, March 16-21, Austin, TX (2003).
- [C94] Fabiano Oyafuso, Gerhard Klimeck, Timothy B. Boykin, R. Chris Bowen, and Paul von Allmen, "Effects of Electronic and Strain Boundary Conditions in Multi-million Atom Electronic Structure Simulations", March Meeting of American Physical Society, March 16-21, Austin, TX (2003)
- [C93] Timothy B. Boykin, Gerhard Klimeck, R. Chris Bowen, and Fabiano Oyafuso, "Diagonal parameter shifts in strained semiconductors in the empirical tight-binding theory", March Meeting of American Physical Society, March 16-21, Austin, TX (2003).
- [C92] Gerhard Klimeck, Fabiano Oyafuso, R. Chris Bowen, Timothy B. Boykin, and Paul von Allmen, "NEMO 3-D: Multi-Million Atom Electronic Structure Calculation, Simulation of Alloy Disorder in Quantum Dots", The NASA University Research, Engineering, and Technology Institute for Nanoelectronics and Computing (INAC) and The NSF Network for Computational Nanotechnology (NCN), Official Kickoffs and Workshop, Purdue University, West Lafayette, IN, Jan. 15-17, 2003.
- [C91] Paul von Allmen and Gerhard Klimeck, "Transport simulation of precessing spin distribution across semiconductor heterojunctions", Materials Research Society Meeting, Boston, MA, Dec 1-6, 2002.
- [C90] Gerhard Klimeck, "NEMO: A User-friendly Quantum Device Design Tool", Twenty-Five Years Ultra-Small Electronics Research, Larry Cooper Symposium, November 29, 2002, Hapuna Beach, Hawaii.
- [C89] Gerhard Klimeck, Fabiano Oyafuso, Chris Bowen, Paul von Allmen, Tom Cwik, Ed Vinyard, Edith Huang, Tim Boykin "Quantum Dot Modeling using NEMO 3-D: IT Challenges in the development of quantum device simulator", JPL representation in the NASA booth of Supercomputing 2002, Baltimore, MD, Nov 17-22, 2002.
- [C88] Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, Tim Boykin, Paul von Allmen, "Study of Alloy Induced Disorder in Quantum Dots using Tight-binding", 4th Motorola Workshop on Computational Materials and Electronics, Tempe, AZ, Nov 14-15, 2002.
- [C87] Gerhard Klimeck, Fabiano Oyafuso, Paul von Allmen, "Development of a 3-D tight-binding-based electronic structure simulator for multi-million atom systems NEMO 3-D", SOCAL Southern California Workshop on Parallel Computing, Santa Barbara, CA, Oct. 28, 2002.

- [C86] Akos (Joey) Czikmantory, Tom Cwik, Edward Vinyard, Hook Hua, Fabiano Oyafuso, Gerhard Klimeck, "WIGLAF A Web Interface Generator and Legacy Application Facade", 2nd JPL IT Symposium, Pasadena, CA, Nov 4, 2002.
- [C85] Paul von Allmen, Gerhard Klimeck, and Fabiano Oyafuso, "Simulation of the electric field dependent spin dynamics in semiconductor thin films", 2nd JPL IT Symposium, Pasadena, CA, Nov 4, 2002.
- [C84] Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, Tim Boykin, Paul von Allmen, "Modeling of Disordered Multimillion Atom Quantum Dot Systems", 2nd JPL IT Symposium, Pasadena, CA, Nov 4, 2002.
- [C83] Gerhard Klimeck, Gary Yagi, Robert Deen, Myche McAuley, Eric DeJong, Fabiano Oyafuso, "Image Correlation Quality Control enabled by Cluster Computing", 2nd JPL IT Symposium, Pasadena, CA, Nov 4, 2002...
- [C82] Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, Timothy B. Boykin, and Paul von Allmen, "Boundary Conditions in Disordered Multimillion Atom Quantum Dot Systems", 2nd International Conference on Semiconductor Quantum Dots -QD2002-, September 30 - October 3, 2002 Komaba Campus, University of Tokyo.
- [C81] Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Nanoelectronic 3-D (NEMO 3-D) Simulation of Multimillion Atom Quantum Dot Systems", SISPAD 2002, Kobe, Japan, Sept. 3-6, 2002.
- [C80] Gerhard Klimeck, Fabiano Oyafuso, E. Bob Tisdale, Akos Czikmantory, "Eigensolver and Cluster Middleware Development", Computational Technology Project Meeting, NASA Goddard Space flight center, MD, July 10, 2002.
- [C79] Gerhard Klimeck and Thomas A. Cwik, "GENES: Genetically Engineered Nanostructures", Nanospace 2002, Galveston, TX, June 24-28, 2002.
- [C78] Paul von Allmen and Gerhard Klimeck, "Transport Simulation of Precessing Spin Distribution across Semiconductor Heterojunctions", Nanospace 2002, Galveston, TX, June 24-28, 2002.
- [C77] Gerhard Klimeck, Fabiano Oyafuso, Timothy B. Boykin, and R. Chris Bowen, "Quantum Dot Simulation", AFRL-JPL workshop on Nanotechnology, Pasadena, CA, May 8-10, 2002.
- [C76] Myche McAuley, Gerhard Klimeck, Bob Deen, Tom Cwik, Eric DeJong, "Mars Image Processing on Commodity Cluster Computers", Science Data Processing Session, 4th Quality Mission Software Workshop, Dana Point, CA, May 7-8 2002.
- [C75] Gerhard Klimeck, "JPL interaction with the proposed NSF funded Network for Computational Nanotechnology", Workshop on a National Network for Nanoscale Modeling and Simulation, Sponsored by the National Science Foundation, Purdue University, April 11, 2002...
- [C74] Gerhard Klimeck, Fabiano Oyafuso, Timothy B. Boykin, and R. Chris Bowen, "Multi-million Atom Electronic Structure Simulations using NEMO 3-D", March Meeting of American Physical Society, March 17-22, Indianapolis, IN (2002)
- [C73] Seungwon Lee, Lars Jönsson, Jeongnim Kim, John W. Wilkins, Garnett W. Bryant, and Gerhard Klimeck, "Many-body interactions in multiply-charged quantum dots modeled by empirical tight-binding", March Meeting of American Physical Society, March 17-22, Indianapolis, IN (2002)
- [C72] Gerhard Klimeck, "A GA practitioner's view on what is needed for efficient use of a 1000 CPU cluster", JPL Workshop on Evolvable Systems, Feb 25, 2002

- [C71] Gerhard Klimeck "Full Brillouin-Zone, Charge Self-consistent Quantum Transport Simulation Enabled by Parallelization of the Nanoelectronic Modeling Tool (NEMO 1-D) on a Beowulf Cluster", 8th International Workshop on Computational Electronics, October 15-18, 2001, Univ. of Illinois, Urbana Champaign.
- [C70] Fabiano Oyafuso, Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Atomistic Electronic Structure Calculations of Unstrained Alloyed Systems Consisting of a Million Atoms", 8th International Workshop on Computational Electronics, October 15-18, 2001, Univ. of Illinois, Urbana Champaign.
- [C69] Tom Cwik, Gerhard Klimeck, Myche McAuley, Bob Deen and Eric Dejong, "Applications on High Performance Cluster Computers Production of Mars Panoramic Mosaic Images", 2001 AMOS Technical Conference, September 10-14, 2001, Maui.
- [C68] Tom Cwik, Gerhard Klimeck, Charles Norton, Thomas Sterling, Frank Villegas and Ping Wang "The Use of Cluster Computers Systems for NASA/JPL Applications", AIAA Space 2001 Conference and Exposition Albuquerque, New Mexico 28-30, August 2001.
- [C67] Tom Cwik, Gerhard Klimeck, and Frank Villegas, "Large-Scale Design and Optimization Using Cluster Computers", IEEE AP-S International Symposium and USNC/URSI National Radio Science Symposium", Boston, MA, July 8-13 (2001).
- [C66] Gerhard Klimeck, Fabiano Oyafuso, R. Chris Bowen, R. Chris Bowen, Timothy B. Boykin, Thomas A. Cwik, Edith Huang, Edward Vinyard "Quantum Dot Modeling using NEMO 3-D, or Development of a Bottom-Up Nanoelectronic Simulator", Sackler Colloquium, National Academy of Sciences, Washington DC, May 18-20 (2001).
- [C65] Gerhard Klimeck, R. Chris Bowen, Fabiano Oyafuso, Tom Cwik, Section 385, Edith Huang, Section 366, "IT Challenges in Nanoscale Electronic Devices Modeling", JPL IT Symposium, Pasadena, CA, May 9 (2001),
- [C64] Gerhard Klimeck, Myche McAuley, Tom Cwik, Bob Deen, Eric DeJong, "Beowulf Processing for Real-time Mission Science and Operations Products", JPL IT Symposium, Pasadena, CA, May 9 (2001).
- [C63] Tom Cwik, Viktor Decyk, Daniel S. Katz, Gerhard Klimeck, Nooshin Meshkaty, Charles Norton, Fabiano Oyafuso, Paul Springer, Thomas Sterling, Bob Tisdale, Frank Villegas, Ed Vinyard, Ping Wang, High Performance Computing Group, "The Use of Cluster Computer Systems for NASA/JPL Applications", Section 385, JPL IT Symposium, Pasadena, CA, May 9 (2001),
- [C62] Gerhard Klimeck, R. Chris Bowen, Timothy B. Boykin, and Fabiano Oyafuso, "Atomistic Quantum Dot Simulation using NEMO-3D", Nanospace 2001, Galveston, Texas, March 13-16 (2001).
- [C61] Lars Jönsson, Seungwon Lee, John W. Wilkins, Garnett W. Bryant, and Gerhard Klimeck, "Sensitivity of electron-hole integrals to choice of atomic orbitals in tight-binding models for nanocrystals.", March Meeting of American Physical Society, March 12-16, Seattle, WA (2001),
- [C60] Timothy B. Boykin, Gerhard Klimeck, and R. Chris Bowen, "A tiger by the tail: the momentum operator in tight-binding", March Meeting of American Physical Society, March 12-16, Seattle, WA (2001),
- [C59] Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Quantum Dot Modeling using NEMO 3-D", March Meeting of American Physical Society, March 12-16, Seattle, WA (2001),
- [C58] Seungwon Lee, Lars Jönsson, John W. Wilkins, Garnett W. Bryant, and Gerhard Klimeck, "Longrange electron-hole exchange in semiconductor quantum dots", March Meeting of American Physical Society, March 12-16, Seattle, WA (2001).

- [C57] D. Keymeulen, Gerhard Klimeck, R. Zebulum, Adrian Stoica, Yili Jin, Carlos-Salazar Lazaro, "EHWPack: an Evolvable Hardware Environment using the Spice Simulator and the Field Programmable Transistor Array", ANNIE12000 (Smart Engineering System Design), St. Louis, MO, November 5-8, 2000.
- [C56] Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Full Band Simulation of Hole Transport in 1-D Heterostructures", 27th international Symposium on Compound Semiconductors (ISCS), IEEE, (2000), Monterey, CA, Oct 2-5 (2000),
- [C55] Didier Keymeulen, Gerhard Klimeck, Ricardo Zebulum, Adrian Stoica, and Carlos Salazar-Lazaro, "EHWPack: A Parallel Software/Hardware Environment for Evolvable Hardware", Genetic and Evolutionary Computation Conference (GECCO-2000), July 8-12, 2000, Las Vegas, Nevada USA.
- [C54] Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Atomistic Simulation of Quantum Dots Including Strain and Bandstructure", Electronic Materials Conference, Denver, CO, June 21-23, 2000.
- [C53] Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Atomistic Simulation of Quantum Dots Including Strain and Bandstructure and Full Band Simulation of Hole Transport in 1-D Heterostructures", International Workshop on Computational Electronics, Glasgow, Scotland, UK, May 22-25, 2000,.
- [C52] Gerhard Klimeck, R. Chris Bowen, Timothy B. Boykin, and Tom Cwik, "sp3s\* and sp3d5s\* Tight-Binding Parameter Sets for GaAs, AlAs, InAs, GaSb, AlSb, InSb, GaP, AlP, and InP for quantum dot simulations", March Meeting of the American Physical Society, Minneapolis, MN, March 20-24, 2000,
- [C51] Gerhard Klimeck, R. Chris Bowen, Tom Cwik, and Timothy B. Boykin, "A Prototype of a 3-D Nanoelectronic Modeling Tool (NEMO-3D)", Nanospace 2000, Houston, TX Jan. 23-28, 2000.
- [C50] Timothy B. Boykin, Gerhard Klimeck, and R. Chris Bowen, "Nanoelectronic Device Calculation from an atomistic point of view: Empirical Tight-Binding Models for Semiconductor Heterostructures", Nanospace 2000, Houston, TX Jan. 23-28, 2000.
- [C49] Gerhard Klimeck, R. Chris Bowen, and Timothy B. Boykin, "Development of a 3-D Nanoelectronic Modeling Tool (NEMO-3D)", Surfaces and Interfaces in Mesoscopic Devices, Maui, Hawaii, Dec. 5-10, 1999.
- [C48] Gerhard Klimeck and R. Chris Bowen, "Nanoelectronic Modeling (NEMO 1-D and NEMO 3-D)", Supercomputing 99, Portland Oregon, Nov. 13-19, 1999, demo exhibit in NASA booth.
- [C47] Tom Cwik and Gerhard Klimeck, "Genetically Engineered Microelectronic Infrared Filters", First NASA/DoD Workshop on Evolvable Hardware, July 19-21, 1999, Pasadena, CA.
- [C46] Gerhard Klimeck, Carlos H. Salazar-Lazaro, Adrian Stoica, and Tom Cwik, "Genetically Engineered Nanoelectronics", First NASA/DoD Workshop on Evolvable Hardware, July 19-21, 1999, Pasadena, CA.
- [C45] Adrian Stoica, Gerhard Klimeck, Carlos Salazar-Lazaro, Didier Keymeulen, and Anil Thakoor, "Evolutionary design of electronic devices and circuits", 1999 Congress on Evolutionary Computation, Washington, D.C. July 6-9, 1999.
- [C44] Tom Cwik and Gerhard Klimeck, "Optimization of Microelectronic Devices for Sensor Applications", Micro and NanoTechnology 99, Pasadena, CA, April 12, 1999.
- [C43] Timothy B. Boykin, Lisa J. Gamble, Gerhard Klimeck, R. Chris Bowen, "Valence-band warping in tight-binding models and its effect on heterostructure electronic states", American Physical Society Centennial Meeting, March 22-26, Atlanta, GA (1999).

- [C42] Gerhard Klimeck, R. Chris Bowen, Tom Cwik, and Timothy B. Boykin, "Tight Binding sp3s\* Material Parameters from Genetic Algorithms", American Physical Society Centennial Meeting, March 22-26, Atlanta, GA (1999).
- [C41] Tom Cwik and Gerhard Klimeck, "Integrated Design and Optimization of Microelectronic Devices", IEEE Aerospace Conference, March 15-19, 1999, Aspen, CO.
- [C40] Gerhard Klimeck, Carlos H. Salazar-Lazaro, Adrian Stoica, Tom Cwik, and Timothy B. Boykin, "Material Parameter Analysis using quantum mechanical electron transport simulations and genetic algorithms", Material Research Society Meeting, Symposium JJ, Materials in Space Science, Technology, and Exploration November 29 December 2, 1998, Boston MA.
- [C39] Gerhard Klimeck, Carlos H. Salazar-Lazaro, Adrian Stoica, Tom Cwik, "Genetically Engineered Nanostructure Device", NanoSpace98, International Conference on Integrated Nano/Microtechnology for Space Applications. Nov. 1-6, 1998, Houston, TX.

## CONTRIBUTED CONFERENCES (WORK PERFORMED PRIOR TO JPL)

- [C38] Gerhard Klimeck, Daniel K. Blanks, Roger Lake, Timothy B. Boykin, R. Chris Bowen, "NEMO: A 1-D Heterostructure Design Tool", March Meeting of the American Physical Society, March 16-20, Los Angeles, CA (1998).
- [C37] Timothy B. Boykin, Gerhard Klimeck, Roger Lake, and R. Chris Bowen, "The Well-Tempered Tight-Binding Model: Many Parameters Do Not Necessarily Imply Flexibility", March Meeting of the American Physical Society, March 16-20, Los Angeles, CA (1998).
- [C36] Harold Grubin, Gerhard Klimeck, and Daniel K. Blanks, "NEMO-PC", 1997 DARPA ULTRA Electronics and Advanced Microelectronics Program Review, October 26-31, Santa Fe, NM (1998).
- [C35] Gerhard Klimeck, Roger Lake and Daniel K. Blanks, "Numerical Approximations to the Treatment of Interface Roughness Scattering in Resonant Tunneling Diodes", Surfaces and Interfaces of Mesoscopic Devices, December 7-12, 1997, Kaanapali, Maui, Hawaii.
- [C34] Roger Lake, Gerhard Klimeck and Daniel K. Blanks, "Interface Roughness and Polar Optical Phonon Scattering in InGaAs/AlAs/InAs RTDs", Surfaces and Interfaces of Mesoscopic Devices, December 7-12, 1997, Kaanapali, Maui, Hawaii.
- [C33] R. Chris Bowen, Chenjing L. Fernando, Gerhard Klimeck, Amitava Chatterjee, Dan Blanks, Roger Lake, Jerry Hu, Joseph Davis, Mak Kulkarni, Sunil Hattangady, and Ih-Chin Chen, "Physical Oxide Thickness extraction and Verification using Quantum Mechanical Simulation", IEEE IEDM, Washington, DC, Dec. 8-10 1997.
- [C32] J. P. A. van der Wagt, A. C. Seabaugh, Gerhard Klimeck, E. A. Beam III., T. B. Boykin, R. C. Bowen, and R. Lake, "Ultralow current density RTDs for tunneling-based SRAM", IEEE International Symposium on Compound Semiconductors, San Diego, CA, Sept. 8-11 1997.
- [C31] Roger Lake, Berinder Brar, Glen D. Wilk, Alan C. Seabaugh, and Gerhard Klimeck, "Resonant Tunneling in Disordered Systems such as SiO2/Si/SiO2", IEEE International Symposium on Compound Semiconductors, San Diego, CA, Sept. 8-11 1997.
- [C30] Daniel K. Blanks, Gerhard Klimeck, Roger Lake, R. Chris Bowen, Manhua Leng, Chenjing Fernando, William R. Frensley, Dejan Jovanovic, NEMO: General Release of a New Comprehensive Quantum Device Simulator", IEEE International Symposium on Compound Semiconductors, San Diego, CA, Sept. 8-11 1997.
- [C29] Gerhard Klimeck, Roger Lake, R. Chris Bowen, Dan Blanks, Timothy B. Boykin, Manhua Leng, Chenjing Fernando, Dejan Jovanovic, William R. Frensley, Ted Moise, and Y. C. Kao, "The effects of self-consistent charging, incoherent scattering and realistic bandstructure on the non-equilibrium transport of electrons in resonant tunneling diodes.", Non-equilibrium Carrier Dynamics in Semiconductors (HCIS-10) Berlin Germany July 28 August 1 1997

- [C28] Roger Lake, Gerhard Klimeck, R. Chris Bowen, and Dejan Jovanovic, "Numerical Modeling of Non-Equilibrium Incoherent Scattering in Quantum Devices", Non-equilibrium Carrier Dynamics in Semiconductors (HCIS-10), Berlin, Germany, July 28 August 1 1997.
- [C27] Gerhard Klimeck, Timothy B. Boykin, R. Chris Bowen, Roger Lake, Dan Blanks, Ted Moise, Y. C. Kao, and William R. Frensley, "Quantitative Simulation of Strained InP-Based Resonant Tunneling Diodes", The 1997 55<sup>th</sup> IEEE Device Research Conference Digest, IEEE, NJ (1997).
- [C26] Gerhard Klimeck, Roger Lake, R. Chris Bowen, Dan Blanks, Manhua Leng, Chenjing Fernando, William R. Frensley and Dejan Jovanovic, "NEMO: A General Purpose 1-D Quantum Device Simulator", Texas Instruments Corporate Research and Development Conference Aug. 19-20, 1996.
- [C25] Roger Lake, Gerhard Klimeck, "Experimentally Verified Quantum Device Simulations Based on Multiband Models, Hartree Self-consistency, and Scattering Assisted Charging", Proceedings of the 1996 54th IEEE Device Research Conference, Santa Barbara, CA, June 24-26, 1996.
- [C24] Gerhard Klimeck, R. Chris Bowen, Roger Lake, Daniel Blanks, Manhua Leng, Dejan Jovanovic, Chenjing Fernando, William R. Frensley, and Paul Sotirelis, "NEMO: A General Purpose 1-D Quantum Device Simulator", International Conference on Quantum Devices and Circuits, Alexandria, Egypt, June 4-8, 1996.
- [C23] Dan Blanks, Gerhard Klimeck, Roger Lake, Manhua Leng, Dejan Jovanovic, Paul Sotirelis, "NEMO", March Meeting of the American Physical Society, St. Louis, March 1996.
- [C22] Roger K. Lake, Gerhard Klimeck, Chenjing L. Fernando, R. Chris Bowen, Ted Moise and Y. C. Kao, "Interface Roughness and Polar Optical Phonon Scattering in Resonant Tunneling Devices", Third International Symposium on new Phenomena in Mesoscopic Structures, Maui, HI, Dec. 4-8, 1995.
- [C21] Gerhard Klimeck, Roger Lake, R. Chris Bowen, Chenjing L. Fernando and William R. Frensley, "Energy Grid Generation for Resolving and Integrating Ultra-Fine Resonances in Quantum Device Simulation", International Workshop on Computational Electronics, Tempe, AZ, Oct. 30 Nov. 2, 1995.
- [C20] Roger Lake, Gerhard Klimeck, R. Chris Bowen, Dejan Jovanovic, Paul Sotirelis and William R. Frensley, "A Generalized Tunneling Formula for Quantum Device Modeling", Tempe, AZ, International Workshop on Computational Electronics, Oct. 30 Nov. 2, 1995.
- [C19] Dejan Jovanovic, Roger Lake, Gerhard Klimeck, Dan Blanks, Paul Sotirelis, R. Chris Bowen, Chenjing Fernando, and Manhua Leng, "Quantum Mechanical Simulation Tools For Semiconductor Devices", Texas Instruments Corporate Research and Development Conference, Aug. 1995
- [C18] R. Chris Bowen, William R. Frensley and Gerhard Klimeck, "Efficient Multiband I-V simulations for quantum devices", IEEE Cornell Device Conference, Ithaca, NY Aug. 7-9, 1995.
- [C17] Gerhard Klimeck, Roger Lake, R. Chris Bowen, William R. Frensley and Daniel Blanks, "Nanoelectronic Modeling (NEMO)", 1995 53rd Device Research Conference, Charlottesville, VA, June 19-21, 1995.
- [C16] William R. Frensley, Chenjing L. Fernando, R. Chris Bowen, and Gerhard Klimeck, "Modeling Tools for the Development of Quantum and Conventional Semiconductor Heterostructure Devices", Government Microcircuit Application Conference, San Diego, CA, Nov. 1994.
- [C15] Gerhard Klimeck, Roger Lake, R. Chris Bowen, William R. Frensley, "Treatment of Continuum and Discrete Quantum States in the Leads of Resonant Tunneling Diodes", March meeting of the American Physical Society, San Jose, March 19-24, 1994.

- [C14] Gerhard Klimeck, Roger Lake, and Supriyo Datta, "The Phonon Peak in Resonant Tunneling Diodes", Second International Symposium on Quantum Confinement, Electrochemical Society, San Francisco, May 22-27, 1994.
- [C13] Gerhard Klimeck, Roger Lake, Supriyo Datta, and Garnett Bryant, "High Bias Transport through Quantum Dots", Second International Symposium on Quantum Confinement, Electrochemical Society, San Francisco, May 22-27, 1994.
- [C12] Gerhard Klimeck, Roger Lake, Supriyo Datta, and Garnett Bryant, "High Bias Transport through Quantum Dots", Workshop on Surfaces and Interfaces, Hawaii, April 24-29, 1994.
- [C11] Gerhard Klimeck, Roger Lake, Garnett. W. Bryant, and Supriyo Datta, "High Bias Transport through Quantum Dots", March meeting of the American Physical Society, Pittsburgh, March 20-25, 1994.
- [C10] Gerhard Klimeck, Guanlong Chen, and Supriyo Datta, "Conductance Spectroscopy in Coupled Quantum Dots", March meeting of the American Physical Society, Pittsburgh, March 20-25, 1994.
- [C9] Gerhard Klimeck, Guanlong Chen, Roger Lake, and Supriyo Datta "Quantum Transport in Single and Coupled Quantum Dots", Texas Instruments Quantum Device Modeling Workshop, Dallas, Feb. 4-6, 1994.
- [C8] Supriyo Datta, Gerhard Klimeck, and Roger Lake, "Two Approaches to Resonant-Tunneling with Inelastic Scattering: A Comparison", March meeting of the American Physical Society, Seattle, March 22-26, 1993.
- [C7] Roger Lake, Gerhard Klimeck, and Supriyo Datta, "Rate Equations from the Keldysh Formalism Applied to the Phonon Peak in Resonant Tunneling Diodes", March meeting of the American Physical Society, Seattle, March 22-26, 1993.
- [C6] Gerhard Klimeck, Roger Lake, and Supriyo Datta, "Elastic and Inelastic Scattering in the Coulomb Blockade Regime", March meeting of the American Physical Society, Seattle, March 22-26, 1993.
- [C5] Roger Lake, Gerhard Klimeck, and Supriyo Datta, "Rate equations from the Keldysh Formalism Applied to the Phonon Peak in Resonant-Tunneling Diodes" Second International Symposium on "New Phenomena in Mesoscopic Structures", Hawaii, Dec. 7-11, 1992.
- [C4] Gerhard Klimeck, Roger Lake, and Supriyo Datta, "Quantum devices: Where Scattering May Enhance Transport", Purdue Electrical Engineering Industrial Institute Fall Workshop, LED's, HBT's, MBE's, ETC.: What's New in Solid State, October 18-20, 1992.
- [C3] Roger Lake, Gerhard Klimeck, and Supriyo Datta, "A Quantum Device Simulator Based on the Non-Equilibrium Green Function Equations of Keldysh, Kadanoff, and Baym", International Workshop on Computational Electronics, Beckman Institute of the University of Illinois; May 28-29, 1992.
- [C2] Gerhard Klimeck, Ce Chen, Daniel S. Elliott, "Nonlinear Interactions Involving The Real Gaussian Field", Twelfth International Conference on Atomic Physics, University of Michigan, Ann Arbor, July 1990.
- [C1] C. Xie, Gerhard Klimeck, Ce Chen, Daniel S. Elliott, "Nonlinear Interactions Involving The Real Gaussian Field", Optical Society of America Annual Meeting, 1990.

# TECHNICAL REPORTS (WORK PERFORMED AT JPL)

[T20] Gerhard Klimeck, Fabiano Oyafuso, Hook Hua, "XML-based C++ Code Generation for User Interface Integration", Oct. 8, 2002, NTR 30844, JPL New Technology Report.

- [T19] Gerhard Klimeck, E. Robert Tisdale, Fabiano Oyafuso, Hook Hua, "Nanoelectronic Modeling (NEMO 3-D) upgrade to no license restrictions", Oct. 8, 2002, NTR 30843, JPL New Technology Report.
- [T18] Thomas A. Cwik, Akos Czikmantory, Gerhard Klimeck, Fabiano Oyafuso, Hook Hua, Edward S. Vinyard, "WIGLAF (A Web Interface Generator and Legacy Application Façade)", Oct. 8, 2002, NTR 30842, JPL New Technology Report.
- [T17] Gerhard Klimeck, "Structure Based simulator Input using tcl/tk", Oct. 3, 2002, NTR 30835, JPL New Technology Report.
- [T16] Gerhard Klimeck, E. Robert Tisdale, Fabiano Oyafuso, R. Chris Bowen, "Parallel Complex Hermitian Sparse Matrix Eigensolvers", Oct. 3, 2002, NTR 30834, JPL New Technology Report.
- [T15] Gerhard Klimeck, Gary M. Yagi, "Quality Control of Tiepoints Computed from Image Correlation", April 1, 2002, NTR 30632, JPL New Technology Report.
- [T14] Gerhard Klimeck, Robert Deen, Michael McAuley, Eric DeJong, "Parallel Algorithms for Near-Real-time Image Correlation", April 1, 2002, NTR 30631, JPL New Technology Report.
- [T13] Gerhard Klimeck, Robert Deen, Michael McAuley, "Parallel Algorithms for Near-Real-time Mosaic Generation", April 1, 2002, NTR 30630, JPL New Technology Report.
- [T12] Gerhard Klimeck, Fabiano Oyafuso, R. Chris Bowen, Timothy B. Boykin, "Nanoelectronic Modeling 3-D (NEMO 3-D) upgrade", Jan. 6, 2002, NTR 30520, JPL New Technology Report.
- [T11] Gerhard Klimeck, "Tightgen genetic algorithm-based tight binding parameter generation", Oct. 3, 1999, NTR 20877, JPL New Technology Report.
- [T10] Thomas A. Cwik, Gerhard Klimeck, "Integrated Design and Optimization of Microelectronic Devices", Dec. 16, 1998, NTR 20625, JPL New Technology Report.
- [T9] Gerhard Klimeck, "JPL NEMO, Benchmarks including Compiler-Based Parallelization", Sept. 23, 1998, NTR 20552, JPL New Technology Report.
- [T8] Gerhard Klimeck, "JPL NEMO extension for Hole transport", Aug. 1998, JPL New Technology Report.
- [T7] Gerhard Klimeck, "Nanotechnology", Annual report of the Center for Integrated Space Microsystems (CISM) 1999.
- [T6] Gerhard Klimeck, "NEMO Benchmarks on SUN, HP, SGI, and Intel Pentium II", <a href="http://hpc.jpl.nasa.gov/PEP/gekco/parallel/benchmark.html">http://hpc.jpl.nasa.gov/PEP/gekco/parallel/benchmark.html</a> (1998)

## TECHNICAL REPORTS (WORK PERFORMED PRIOR TO JPL)

- [T5] Gerhard Klimeck, Roger Lake, Daniel K. Blanks, "NEMO 3.0 User's, Theory and Technical Guide", Raytheon Corporation, http://www.raytheon.com/rtis/nemo/pubs/nemopubs.htm (1997)
- [T4] Gerhard Klimeck, Roger Lake, Daniel K. Blanks, "NEMO 2.0 User's and Theory Guide", Texas Instruments Incorporated, 1995.
- [T3] Gerhard Klimeck, "Electron-Phonon and Electron-Electron Interactions in Quantum Transport", Technical Report TR-EE 94-7, Purdue University, May 1994.
- [T2] Gerhard Klimeck, Roger Lake, Michael J. McLennan, and Supriyo Datta; "QUEST User's Manual", Technical Report TR-EE 93-17, Purdue University, April 1993.
- [T1] Michael J. McLennan, Gerhard Klimeck and Supriyo Datta, "SQUALID-2D: Version 1.0 and 1.1, A Guide for the User", Technical Report TR-EE 91-15, Purdue University, April 1991.

# INVITED SEMINARS (WORK PERFORMED AT JPL)

- [S37] "Development of NEMO 3-D: Boundary conditions for the electronic structure of finite-extent, embedded semiconductor nanostructures", Gerhard Klimeck, Feb. 27, 2004, Ruhr-University University Bochum, Germany, Host: Prof. Ulrich Kunze.
- [S36] "Development of NEMO 3-D: Boundary conditions for the electronic structure of finite-extent, embedded semiconductor nanostructures", Gerhard Klimeck, Feb. 24, 2004, University of Duisburg-Essen, Germany, Host: Dr. Werner Prost.
- [S35] "Development of the Nanoelectronic Modeling Tool (NEMO): Towards Design, Analysis, Synthesis, and Fundamental Limits", Gerhard Klimeck, Feb. 18, 2004, State University of New York, Buffalo, Host: Prof. Vladimir Mitin.
- [S34] "Computational Nanoelectronics Towards: Design, Analysis, Synthesis, and Fundamental Limits", Gerhard Klimeck, Purdue University, July 28, 2003, Host: Prof. Mark Lundstrom.
- [S33] "Computational Nanoelectronics Towards: Design, Analysis, Synthesis, and Fundamental Limits", Gerhard Klimeck, JPL, Division 32 and 38 Seminar, June 18, Host: Dr. Carl Ruoff, Div 32&38 Chief Technologist.
- [S32] "Computational Nanoelectronics Towards: Design, Analysis, Synthesis, and Fundamental Limits", Gerhard Klimeck, JPL, Section 381 Noontime seminar, April 10, 2003, Host Jason Hyon, Section 381 Deputy.
- [S31] "Computational Nanoelectronics Towards: Design, Analysis, Synthesis, and Fundamental Limits", Gerhard Klimeck, Dr. Ed Stone Award Outstanding Research Publication Award Lecture, JPL, Feb. 18, 2003, Host: Dr. Tom Prince, JPL Chief Scientist.
- [S30] "Modeling of Disordered Multimillion Atom Quantum Dot Systems", Gerhard Klimeck, University of Duisburg, Germany, Nov 13, 2002, Hosts Dr. Werner Prost and Prof. Tegude.
- [S29] "Modeling of Disordered Multimillion Atom Quantum Dot Systems", Gerhard Klimeck, Ruhr-University Bochum, Germany, Nov 11, 2002, Host Prof. Ulrich Kunze.
- [S28] "Development of a Nanoelectronic 3-D (NEMO 3-D) Simulator for Multimillion Atom Simulations and Its Application to Alloyed Quantum Dots", Gerhard Klimeck, California State University Northridge, Northridge, CA, March 29, 2002, Host Prof. Nickolas Kioussis.
- [S27] "Development of a Nanoelectronic 3-D (NEMO 3-D) Simulator for Multimillion Atom Simulations and Its Application to Alloyed Quantum Dots", Gerhard Klimeck, Purdue University, West Lafayette, IN, March 20, 2002, Host Prof. Supriyo Datta.
- [S26] "Development of a Nanoelectronic 3-D (NEMO 3-D) Simulator for Multimillion Atom Simulations and Its Application to Alloyed Quantum Dots", Gerhard Klimeck, Notre Dame, South Bend, IN, March 15, 2002, Host Prof. Wolfgang Porod.
- [S25] "Development of a Nanoelectronic 3-D (NEMO 3-D) Simulator for Multimillion Atom Simulations and Its Application to Alloyed Quantum Dots ", Gerhard Klimeck, University of Wisconsin, Madison, WI, March 14, 2002, Host Prof. Bob Joynt
- [S24] "Status of the Nanoelectronic Modeling tool (NEMO 1-D and 3-D) and its planned extension to Spintronics", Gerhard Klimeck, NTT Central Research Laboratory, Erato Project, Feb 8, 2002, Hosts Dr. Michael Stopa and Prof. Tarucha.
- [S23] "Nanoelectronic Modeling (NEMO): Moving from commercial grade 1-D simulation to prototype 3-D simulation", Gerhard Klimeck, University of Tokyo, February 8, 2002, Host Prof. Seigo Tarucha.
- [S22] "Status of the Nanoelectronic Modeling tool (NEMO 1-D and 3-D) and its planned extension to Spintronics", Gerhard Klimeck, Tokyo Institute of Technology, Feb 6, 2002, Host Prof. Oda.

- [S21] "Nanoelectronic Modeling (NEMO): Moving from commercial grade 1-D simulation to prototype 3-D simulation", Gerhard Klimeck, Osaka University, January 30, 2002, Host Prof. Hishiro Hamaguchi.
- [S20] Gerhard Klimeck, "Quantum Dot Modeling using NEMO 3-D", JPL, Section 367 Seminar, February 6, 2001, 126-346, 3p.m.
- [S19] Gerhard Klimeck, "Quantum Dot Modeling using NEMO 3-D", University of California Riverside, Department of Electrical and Computer Engineering, Dec 8, 2000.
- [S18] Gerhard Klimeck, Chris Bowen, Tom Cwik, and Timothy B. Boykin, "A Prototype of a 3-D Nanoelectronic Modeling Tool (NEMO-3D)", Notre Dame, South Bend, IN, April 12, 2000.
- [S17] Gerhard Klimeck, Chris Bowen, Tom Cwik, and Timothy B. Boykin, "A Prototype of a 3-D Nanoelectronic Modeling Tool (NEMO-3D)", General Dynamics Information Systems, Minneapolis, MN, March 22, 2000.
- [S16] Gerhard Klimeck, Chris Bowen, and Tom Cwik, "Simulator Development for Nanoelectronic and Electromagnetic Devices", National Reconnaissance Office, Chantilly, VA, March 31, 1999.
- [S15] Gerhard Klimeck, Chris Bowen, Tim Boykin, Fabiano Oyafuso, Tom Cwik, Carlos Salazar-Lazaro, and Adrian Stoica, "The Nanoelectronic Modeling Tool NEMO and its extension to High Performance Computing", MIT Lincoln Laboratory, Lexington, MA. Dec. 2, 1998.
- [S14] Gerhard Klimeck, Chris Bowen, Tim Boykin, Fabiano Oyafuso, Tom Cwik, Carlos Salazar-Lazaro, and Adrian Stoica, "The Nanoelectronic Modeling Tool NEMO and its extension to High Performance Computing", Gerhard Mercator University Duisburg, Nov 25, 1998.
- [S13] Gerhard Klimeck, Chris Bowen, Tim Boykin, Fabiano Oyafuso, Tom Cwik, Carlos Salazar-Lazaro, and Adrian Stoica, "The Nanoelectronic Modeling Tool NEMO and its extension to High Performance Computing", Ruhr University Bochum, Lehrstuhl fuer Werkstoffe der Elektrotechnik, Nov 23, 1998.

# INVITED SEMINARS (WORK PERFORMED PRIOR TO JPL)

- [S12] Gerhard Klimeck, "NEMO: A 1-D Heterostructure Design Tool", Center for Integrated Space Microsystems, Jet Propulsion Laboratory, Pasadena, CA, April 24, 1998.
- [S11] Gerhard Klimeck, "NEMO: A General Purpose 1-D Quantum Device Simulator", November 21, 1997, Intel Corporation, Portland, OR.
- [S10] Gerhard Klimeck, "NEMO: A General Purpose 1-D Quantum Device Simulator", October 6, 1997, Jet Propulsion Laboratory, Pasadena, CA.
- [S9] Gerhard Klimeck, "NEMO: Quantitative RTD Simulation", Hitachi Ltd., Cambridge, UK, July 21, 1997.
- [S8] Gerhard Klimeck, Dejan Jovanovic, "NEMO: Quantum Device Modeling (1-D, 2-D and 3-D), Ultra Electronics Program Review, Estes Park, CO, Oct. 6-10, 1996.
- [S7] Gerhard Klimeck, Roger Lake, R. Chris Bowen, Dan Blanks, Manhua Leng, Chenjing Fernando, Dejan Jovanovic, and Paul Sotirelis, "NEMO: A General Purpose Quantum Device Simulator", IMEC, Leuven, Belgium, May 31, 1996.
- [S6] Gerhard Klimeck, Roger Lake, R. Chris Bowen, Dan Blanks, Manhua Leng, Chenjing Fernando, Dejan Jovanovic, and Paul Sotirelis, "NEMO: A General Purpose Quantum Device Simulator", Ruhr-Universität Bochum, Germany, May 30, 1996.
- [S5] Gerhard Klimeck, Roger Lake, R. Chris Bowen, Dan Blanks, Manhua Leng, Chenjing Fernando, Dejan Jovanovic, and Paul Sotirelis, "NEMO: A General Purpose Quantum Device Simulator", Universität Duisburg, Germany, May 28, 1996.

- [S4] Gerhard Klimeck, Roger Lake, R. Chris Bowen, Dan Blanks, Manhua Leng, Chenjing Fernando, Dejan Jovanovic, and Paul Sotirelis, "NEMO: A General Purpose Quantum Device Simulator", Texas Instruments Research Colloquium, Dallas, TX, May 23, 1996.
- [S3] Gerhard Klimeck, Roger Lake, Garnett Bryant, Guanlong Chen, Supriyo Datta, Chris Bowen, William Frensley, "Elektronen-Elektronen und Elektronen-Phononen Wechselwirkungen in der Nanotechnologie", Ruhr-Universität Bochum, Germany, Dec. 20, 1994.
- [S2] Gerhard Klimeck, Roger Lake, Garnett Bryant, Guanlong Chen, Supriyo Datta, Chris Bowen, William R. Frensley, "Elektronen-Elektronen und Elektronen-Phononen Wechselwirkungen in der Nanotechnologie", Universität Duisburg, Germany, Dec. 15, 1994.
- [S1] Gerhard Klimeck, Roger Lake, and Supriyo Datta, "Erhöhter Stromfluss durch Streuprozesse oder Überraschende Ergebnisse im Bereich der Quantenbauelemente", Ruhr-Universität Bochum, Germany, Jan. 8, 1993.

# PROGRAM REVIEWS (WORK PERFORMED AT JPL)

- [R29] Gerhard Klimeck, Timothy B. Boykin, Mark Eriksson, Mark Friesen, Susan Coppersmith, Fabiano Oyafuso, Paul von Allmen, Seungwon Lee, and K. Birgitta Whaley, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", NSA / ARDA / ARO Quantum Computing Technology Workshop, Nashville, TN, August 18-22, 2003.
- [R28] Gerhard Klimeck, Fabiano Oyafuso, Bob Tisdale, Hook Hua, R. Chris Bowen, "Development of a Parallel Eigensystem Solver for Beowulf Clusters", Oct 31 2002, JPL ESTO-CT program review.
- [R27] Gerhard Klimeck, Joey Czikmantory, Hook Hua, "WIGLAF A Web Interface Generator and Legacy Application Facade", Oct 31 2002, JPL ESTO-CT program review.
- [R26] Gerhard Klimeck, Timothy B. Boykin, Fabiano Oyafuso, and Paul von Allmen, "Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates", NSA / ARDA / ARO Quantum Computing Technology Workshop, Nashville, TN, August 19-23, 2002.
- [R25] Nikzad Toomarian, R. Chris Bowen, Gerhard Klimeck, "Quantum Dot Modeling Development of a Bottom-Up Nanoelectronic Modeling Tool", May 9, 2001, JPL CISM (Center for Integrated Space Microelectronics) zero-base review of RCT (Revolutionary Computing Technologies) program.
- [R24] R. Chris Bowen, Gerhard Klimeck, "Quantum Dot Modeling Development of a Bottom-Up Nanoelectronic Modeling Tool", September 2000, JPL CISM (Center for Integrated Space Microelectronics) review of RCT (Revolutionary Computing Technologies) program.
- [R23] R. Chris Bowen, Gerhard Klimeck, "Quantum Dot Modeling Development of a Bottom-Up Nanoelectronic Modeling Tool", August 1 2000, JPL CISM (Center for Integrated Space Microelectronics) review of RCT (Revolutionary Computing Technologies) program.
- [R22] R. Chris Bowen, Gerhard Klimeck, "3-D Quantum Device Simulator Development", March 18. 1999, JPL CISM (Center for Integrated Space Microelectronics) review of RCT (Revolutionary Computing Technologies) program.

# PRESENTATIONS AT PROGRAM REVIEWS (WORK PERFORMED AT TEXAS INSTRUMENTS)

[R1-R21] The National Reconnaissance Office, sponsor of the NEMO program, required a quarterly program review. Prof. David Ferry (ASU), Prof. George Haddad (U. of Michigan), and Dr. Harold Grubin (SRA) were hired as scientific reviewers by the program sponsor. In addition, program managers from other agencies such as ONR, DARPA, and NSA were typically present. The reviews were generally held in the Central Research Lab of Texas Instruments or at the DFW Hilton. Individual presentations listed below lasted typically 25-45 minutes.

[R21] Gerhard Klimeck, "NanoElectronic MOdeling-Software Development Approach", Dec. 1997.

- [R20] Gerhard Klimeck, "Program Status, Activities Overview", May 19, 1997.
- [R19] Gerhard Klimeck, "Software Development Theory", May 19, 1997.
- [R18] Gerhard Klimeck, "Software Demo", May 19, 1997.
- [R17] Dan Blanks, Gerhard Klimeck, "Software / Interface Development", Nov. 1996.
- [R16] Gerhard Klimeck, "Test Matrix Results", Nov. 1996.
- [R15] NEMO Phase I Review in Washington DC, "NEMO Software Summary", May 1996.
- [R14] NEMO Phase I Review in Washington DC, "NEMO Software Tutorial" (3 hours), May 1996.
- [R13] Gerhard Klimeck, "NEMO: Software Development", Feb. 7, 1996.
- [R12] Gerhard Klimeck, "NEMO: GUI Development", Feb. 7, 1996.
- [R11] R. Chris Bowen, Gerhard Klimeck, "Multiband Simulations", Feb. 7, 1996.
- [R10] Gerhard Klimeck, "GUI and Theory Interaction A Dynamic Design"
- [R9] Gerhard Klimeck, "NEGF Code Development", October 11, 1995.
- [R8] R. Chris Bowen, Gerhard Klimeck, "Multiband Simulation Results", October 11, 1995.
- [R7] Gerhard Klimeck, William R. Frensley, Chenjing L. Fernando, R. Chris Bowen, "Non-Equilibrium Green Function Approach Software Development", June 27, 1995.
- [R6] R. Chris Bowen, Gerhard Klimeck, William R. Frensley, "Multiband Simulations", June 27, 1995.
- [R5] Chenjing L. Fernando, Gerhard Klimeck, William R. Frensley, "Polar Optical Phonon Scattering Simulations", June 27, 1995.
- [R4] Gerhard Klimeck, William R. Frensley, Chenjing L. Fernando, R. Chris Bowen, "Non-Equilibrium Green Function Approach Software Development", Feb. 23, 1995.
- [R3] Gerhard Klimeck, William R. Frensley, Chenjing L. Fernando, R. Chris Bowen, "Non-Equilibrium Green Function Approach Software Development", Feb. 23, 1995.
- [R2] Gerhard Klimeck, William R. Frensley, Chenjing L. Fernando, R. Chris Bowen, "Non-Equilibrium Green Function Approach Software Development", fall 1994.
- [R1] William R. Frensley, Gerhard Klimeck, Chenjing L. Fernando, R. Chris Bowen, "Non-Equilibrium Green Function Approach Software Development", summer 1994.