# Semiconductor Device Modeling

**(Applications and Tools)**

**Group Lead: Subhash Saini**

**POC: Bryan Biegel**

## Projects

1. Quasi-classical electronics
2. Nanostructure electronics
3. Atomic chain electronics
4. Quantum optoelectronics

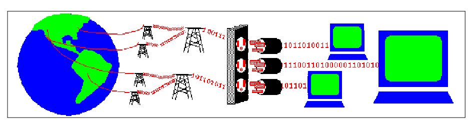
**(Web page: http://www.nas.nasa.gov/Groups/SDM)**

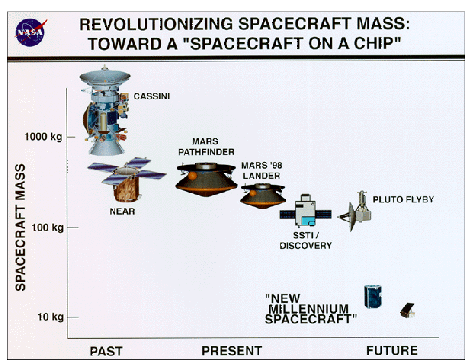


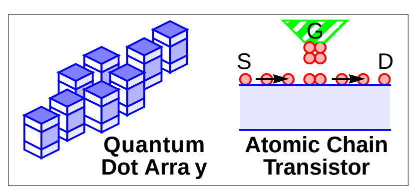
# Why at NASA?

NASA's Interests:

- Future computational power generators
- Space mission requirements:
  - radiation hardness
  - operation dormancy
  - vacuum exposure
  - thermal extremes/cycling
  - acceleration extremes
- Reduce time-to-mission, budget
  - smaller, mechanically simple
  - smarter (autonomous)
- New technologies:
  - molecular/bio/atomic electronics
  - quantum computing
  - quantum optoelectronics



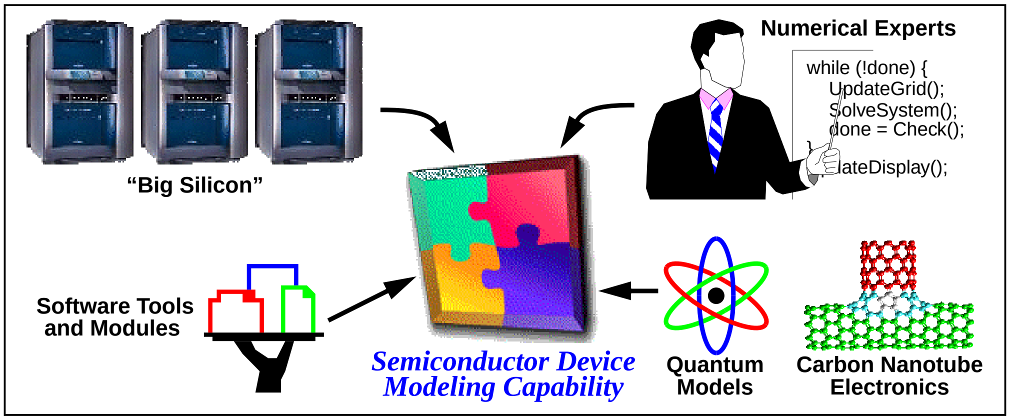


# Why at NAS?

Unique NAS resources make higher goals attainable:

- Supercomputing, parallel computation hardware
- Advanced numerical computation software, experts
- Commitment to computational research (IPG, CoF-IT)
- Critical mass of semiconductor device, nanotechnology expertise

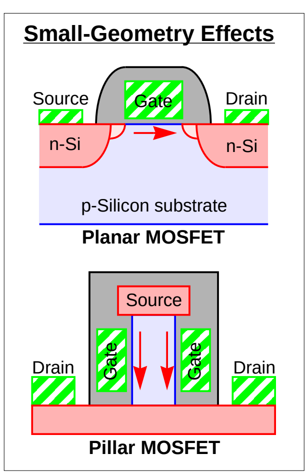


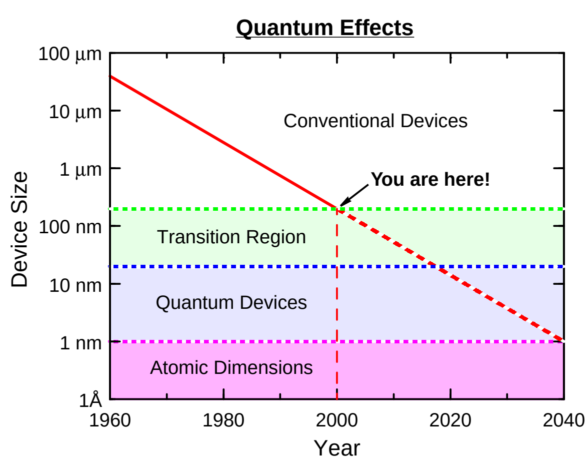



# The Experimental Alternative

Limitations of experimental R&D:

- Expensive, slow, imprecise
- Future technologies not achievable
- Increasingly complicated physics

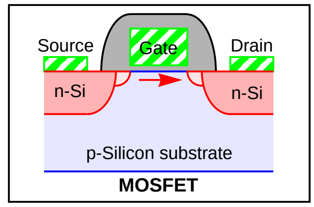


# 1. Quasi-Classical Device Modeling: Overview

Motivation:

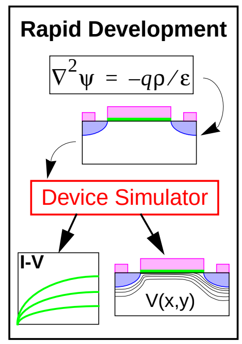
- In near term (< 10 years) MOSFET will dominate electronics
- Quantum effects will increase



MOSFET

Approach:

- Add quantum corrections to conventional models:
  - Drift-diffusion $\Rightarrow$ density-gradient
  - Hydrodynamic $\Rightarrow$ quantum hydrodynamic
  - BTE $\Rightarrow$ Wigner Function transport equation
- Extensible simulation tools; parallel codes
  - PROPHET PDE solver
  - PETSc parallel linear system solver

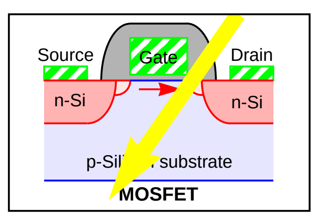





# 1. Quasi-Classical Device Modeling: Plans

1-Year Technical Milestones:

- Accurate mobility, tunneling in classical-quantum model
- Investigate quantum effects in next-generation electronics
- Parallelize, performance-tune simulation tool
- Investigate radiation effects in NASA space electronics



MOSFET

Long-Term Goals:

- NASA mission requirements for conventional electronics
- Advance “Big Silicon” (computational power generators)
- Advance PDE solver approach to rapid model implementation

# 1. Quasi-Classical Device Modeling: Accomplishments

Accomplishments:

- Invited talk, proceedings paper (ultrafast quantum electronics)
- 2 Contributed talks, proceedings (quantum effects in MOSFETs)
- NAS technical report (quantum correction simulation approaches)
- RIACS grant (Internet-based semiconductor device modeling)

Collaborators:

- R.W. Dutton, Z. Yu (Stanford University)
- C.S. Rafferty (Lucent Technologies)
- M.G. Ancona (Naval Research Labs)

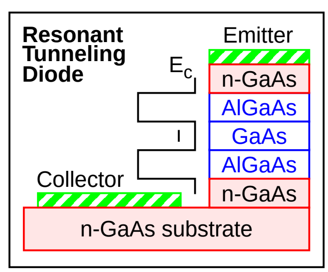
Staff: Bryan Biegel (MRJ)



# 2. Charge Transport in Nanostructures: Overview

Motivation:

- In medium term (10-20 years), conventional devices hit quantum limits
- Quantum nanostructure devices may beat the limits



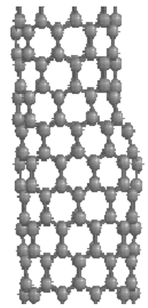

Approach:

- Implement detailed quantum transport model:
  Non-equilibrium Green's functions (NEGF)
- Include phonon scattering, Poisson self-consistency
- Three device types to be studied:
  - ultra-small conventional devices (e.g. sub-100 nm MOSFET)
  - true quantum devices (e.g., RTDs, quantum wires/dots)
  - carbon nanotube devices

# 2. Charge Transport in Nanostructures: Plans

1-Year Technical Milestones:

- Determine feasibility of transient NEGF simulation
- Develop 2-D, steady-state, phase-coherent capability
- Investigate electronic properties of deformed CNTs
- Study transport through molecular structures



Carbon Nanotube Junction

Long-Term Goals:

- Develop quantum electronics for NASA mission goals
  - high compute power/volume for space missions
  - high-speed data/image processing
- Build quantum device simulation expertise at NAS



# 2. Charge Transport in Nanostructures: Accomplishments

Accomplishments:

- 5 peer-reviewed papers (CNT electronics, RTD AC properties, quantum computing)
- Contributed talk (transport in carbon nanotubes)

Collaborators:

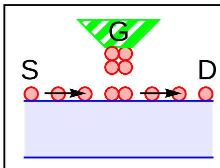
- T.R. Govindan, J. Han (Code IN)
- L. Yang (code ST)
- V.P. Roychowdhury, K.L. Wang (UCLA)

Staff: M.P. Anantram (MRJ)

# 3. Atomic Chain Electronics: Overview

Motivation:

- In long term (> 20 years), bulk fabrication too imprecise for further down-scaling
- atomic-scale electronics is final frontier of miniaturization



Atomic Chain Transistor

Approach:

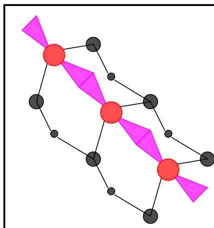
- Investigate band structures of atomically engineered materials:
  - use tight-binding theory with overlap integral
  - find metallic and semiconducting elements
  - determine effects of substrate on chain electronic properties
  - establish doping scheme: geometry and dopants
- Develop atomic-scale transport model including contacts:
  - study semiconductor-metal and p-n junctions
  - predict I-V characteristics of various junctions
- Propose novel, smallest possible electronic devices



# 3. Atomic Chain Electronics: Plans

1-Year Technical Milestones:

- Clarify substrate effects on electronic properties of atomic chains
- Clarify electronic, transport properties of atomic chain junctions
- Study results of As quantum dot chains, closest analog of atomic chain


Atomic Wire Concept

Long-Term Goals:

- Build smallest, lightest electronics for ultra-small NASA applications
- Show how to mimic conventional electronics at atomic dimensions

# 3. Atomic Chain Electronics: Accomplishments

Accomplishments:

- 2 peer-reviewed papers (atomic chain electronics)
- 4 conference talks (doping, electronic properties of atomic chains)
- Patent application (doping method of semiconducting atomic chains)

Collaborators:

- R.A. Kiehl (Stanford University)
- C.W. Bauschlicher, H. Partridge (Code ST)

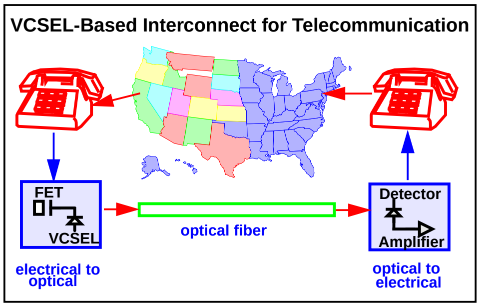
Staff: Toshishige Yamada (MRJ)



# 4. Computational Quantum Optoelectronics: Overview

Motivation:

- Electronic switching, data transmission faces THz limits
- Optoelectronics may beat limits
- Semiconductor optoelectronics can enable new applications



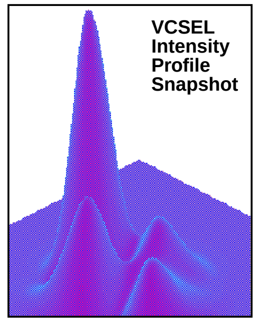

Approach:

- Construct model from microscopic physical processes; use first-principle theories where feasible
- Couple optical, electronic, and thermal processes self-consistently
- Simulate time evolution of models consisting of 2D and/or 3D PDEs
- Collaborate with experimentalists to verify simulations and guide new device designs

# 4. Computational Quantum Optoelectronics: Plans

1-Year Technical Milestones:

- 2-D VCSEL simulation and analysis
- Complete ThZ heating and modulation analysis
- Add thermal processes and plasma heating to VCSEL-code




Long-Term Goals:

- Recommend and support NASA applications of optoelectronics
- Understand optoelectronic physics for THz switching, transmission
- Build comprehensive modeling capabilities for optoelectronics
- Explore optical response of nano-structures, biochemical systems



# 4. Computational Quantum Optoelectronics: Accomplishments

Accomplishments:

- 15 peer-reviewed papers (semiconductor laser and VCSEL modeling, optical pulse propagation)
- 3 invited talks (semiconductor laser theory and modeling)
- 3 contributed talks (semiconductor laser physics)
- DDF grant FY98 (modeling of ultrafast quantum well devices)
- Symposium chair, 2 conference committees

Collaborators:

- J. Li, S. Cheung (Code IN)
- W. Chow (Sandia National Lab)
- J.V. Moloney (University of Arizona)

Staff: Cun-Zheng Ning (MRJ), Peter Goorjian (C.S.)