Nanoelectronic Modeling (NEMO) Motivation and Background

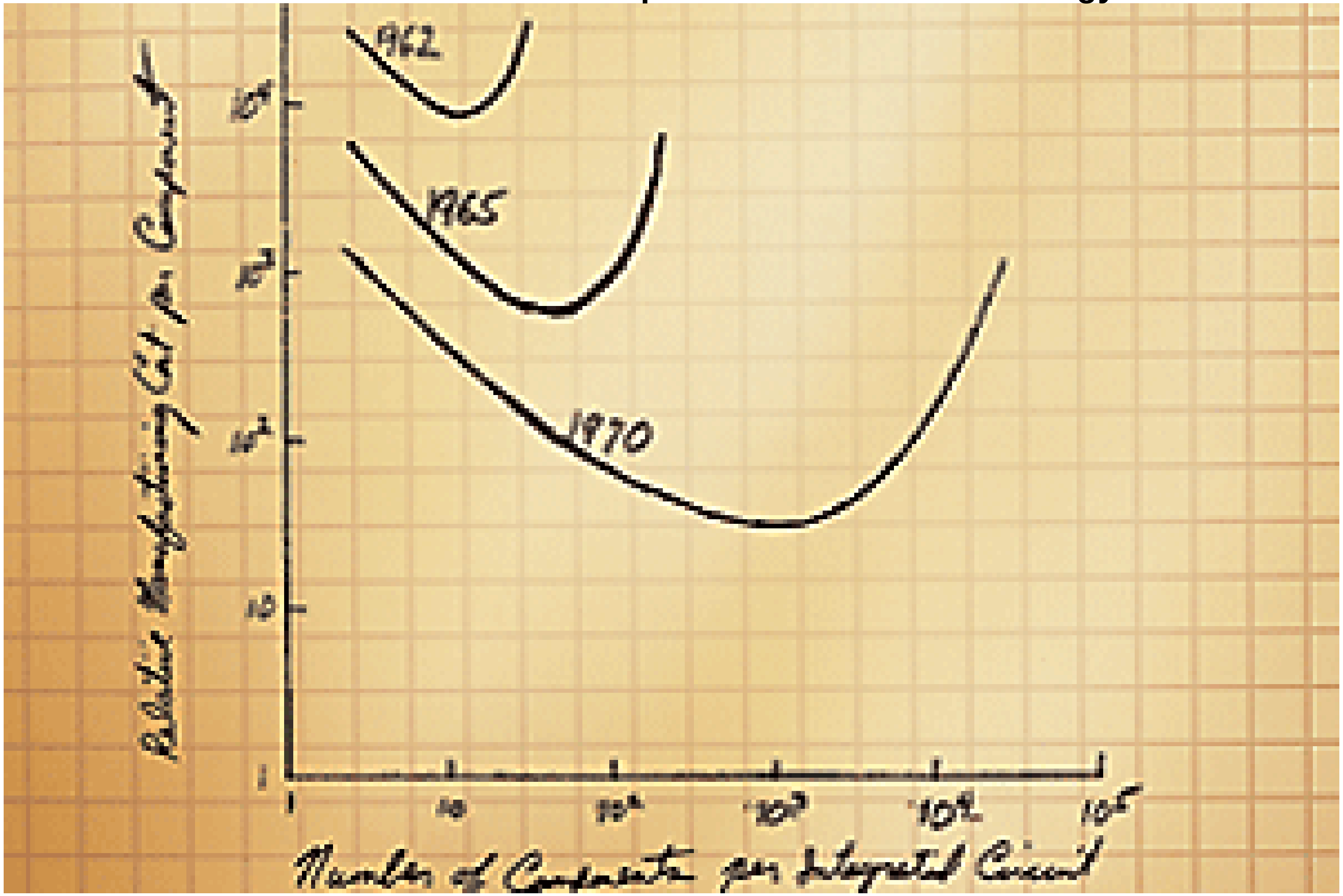
NCN

Gerhard Klimeck
Dragica Vasileska

1965 Gordon Moore => Moore's Law

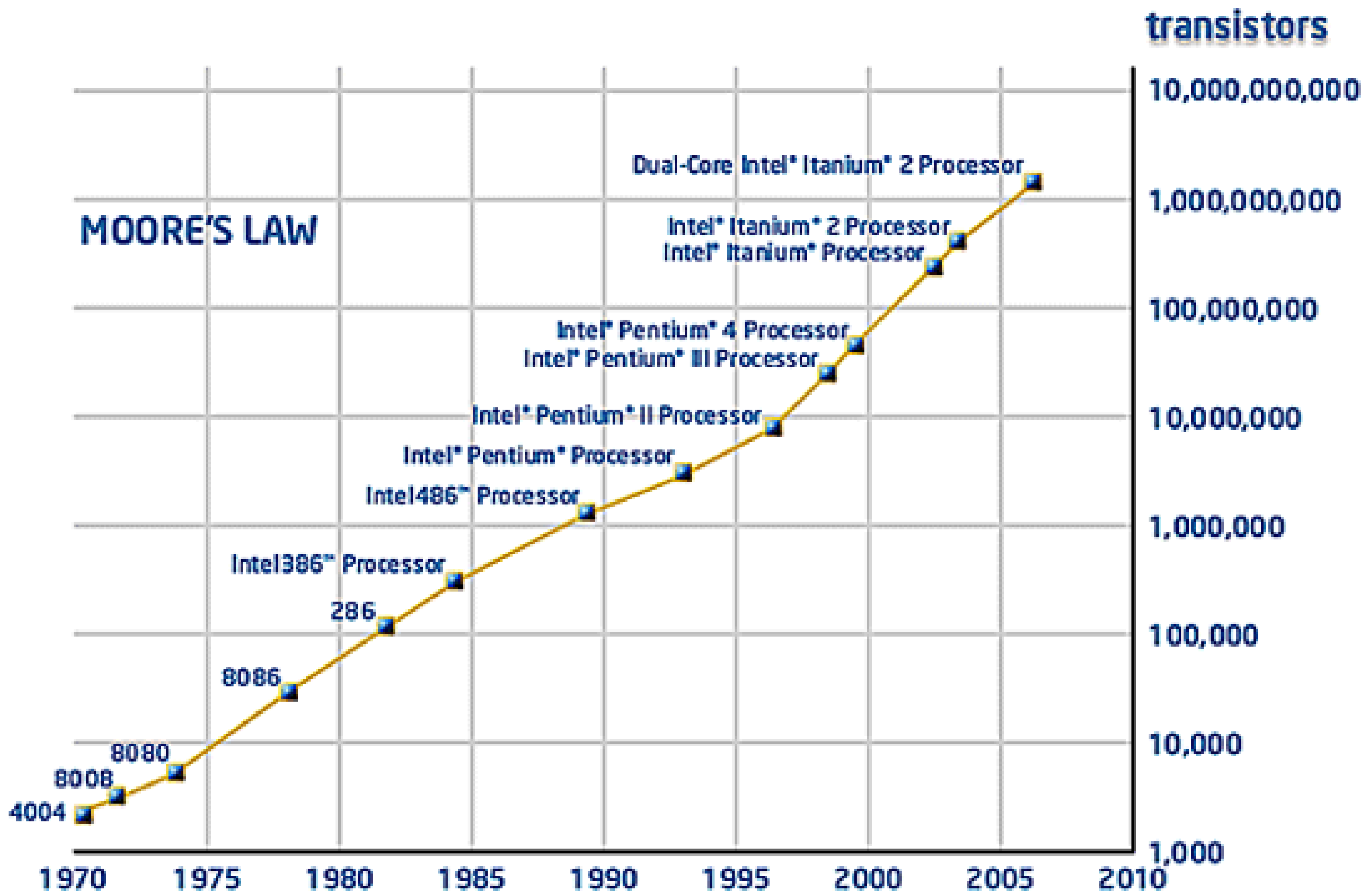
http://www.intel.com/technology/mooreslaw

Relative Manufacturing Cost per Component



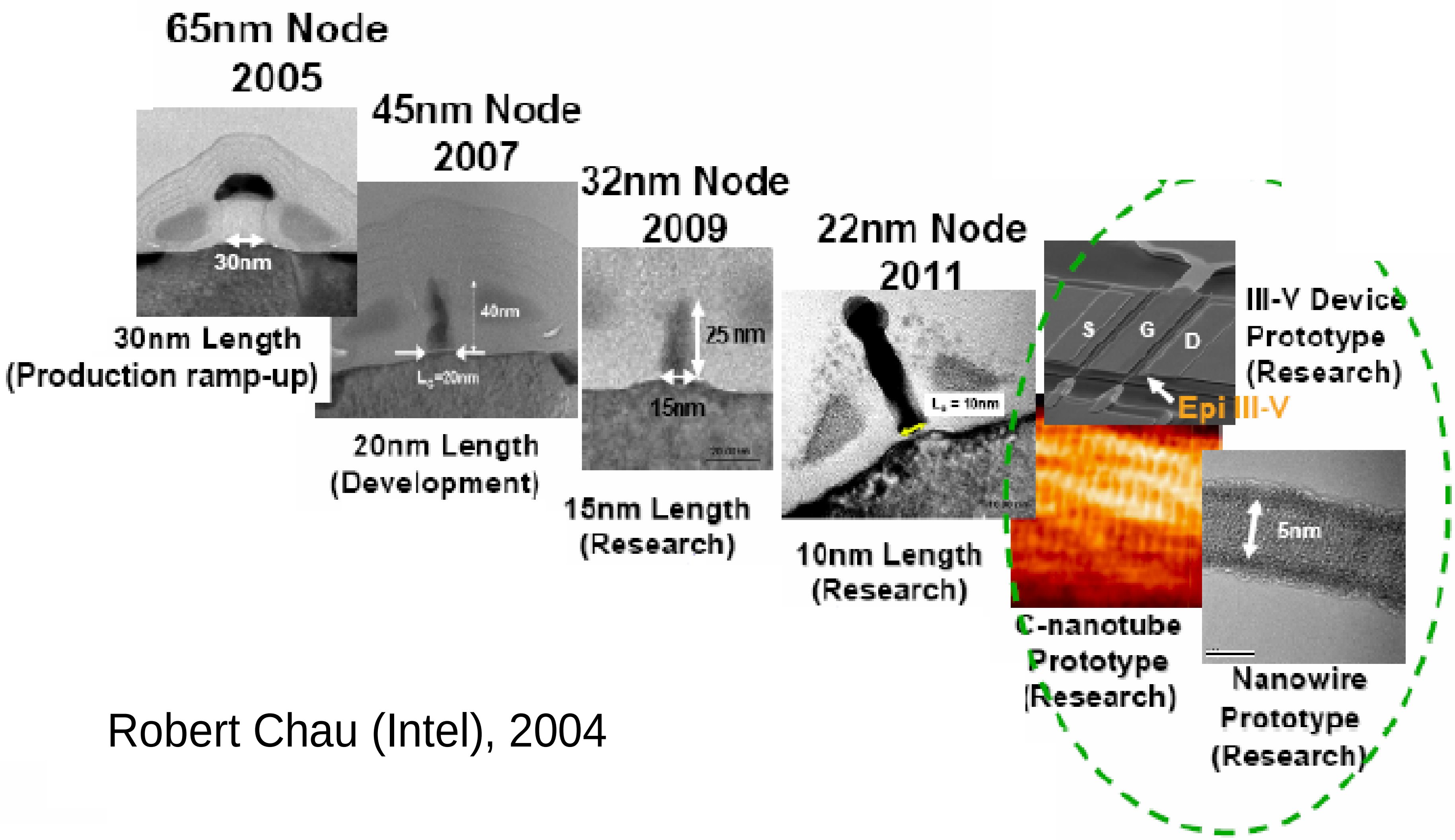
Number of Components per Integrated Circuit nanoHUB online simulation and more — an NCN project

Moore's Law
a Self-Fulfilling Prophesy



- From http://www.intel.com/technology/mooreslaw/index.htm

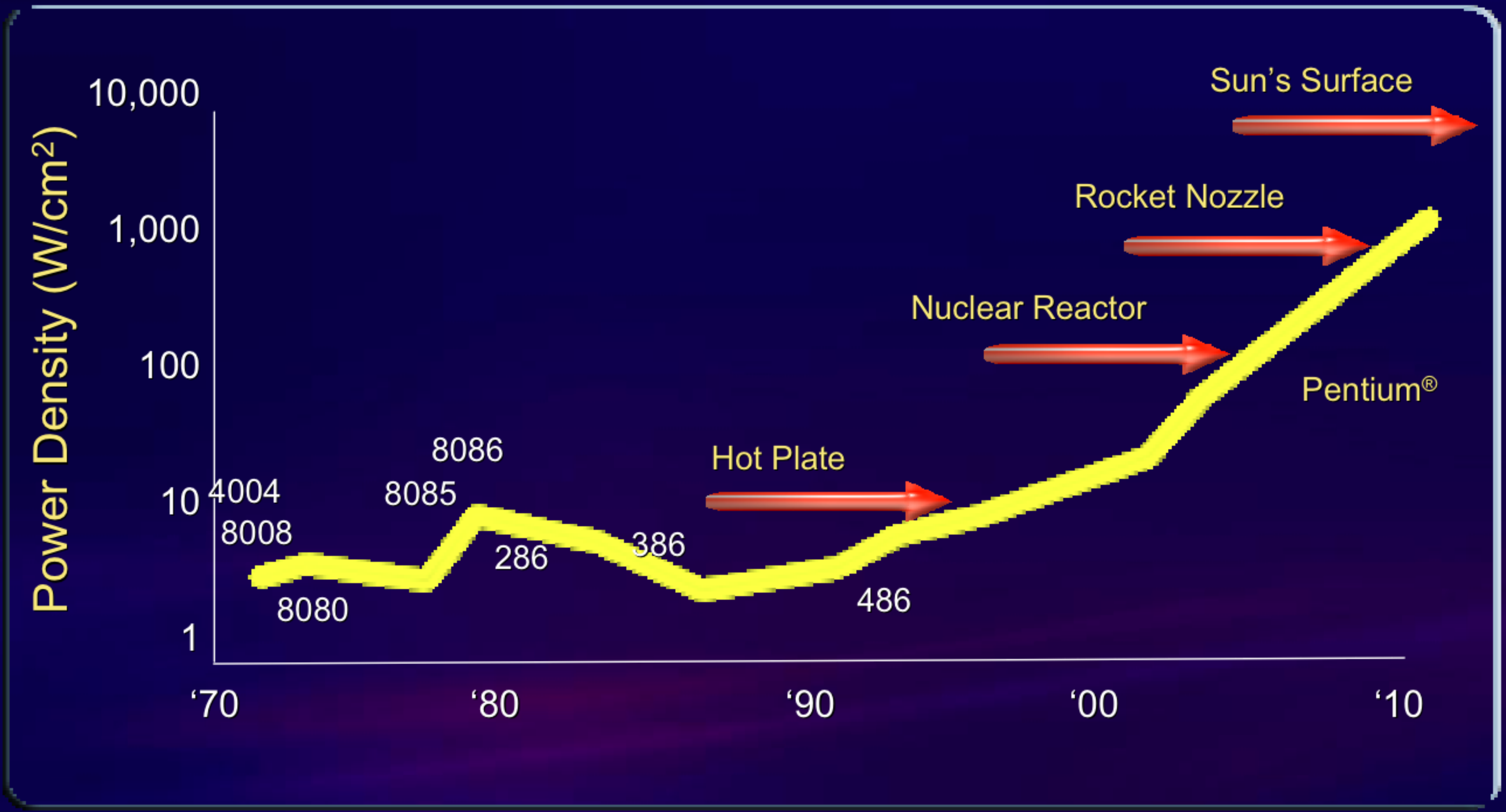
Technical Developments to enable Moore's Law



Robert Chau (Intel), 2004

Today's CPU Architecture

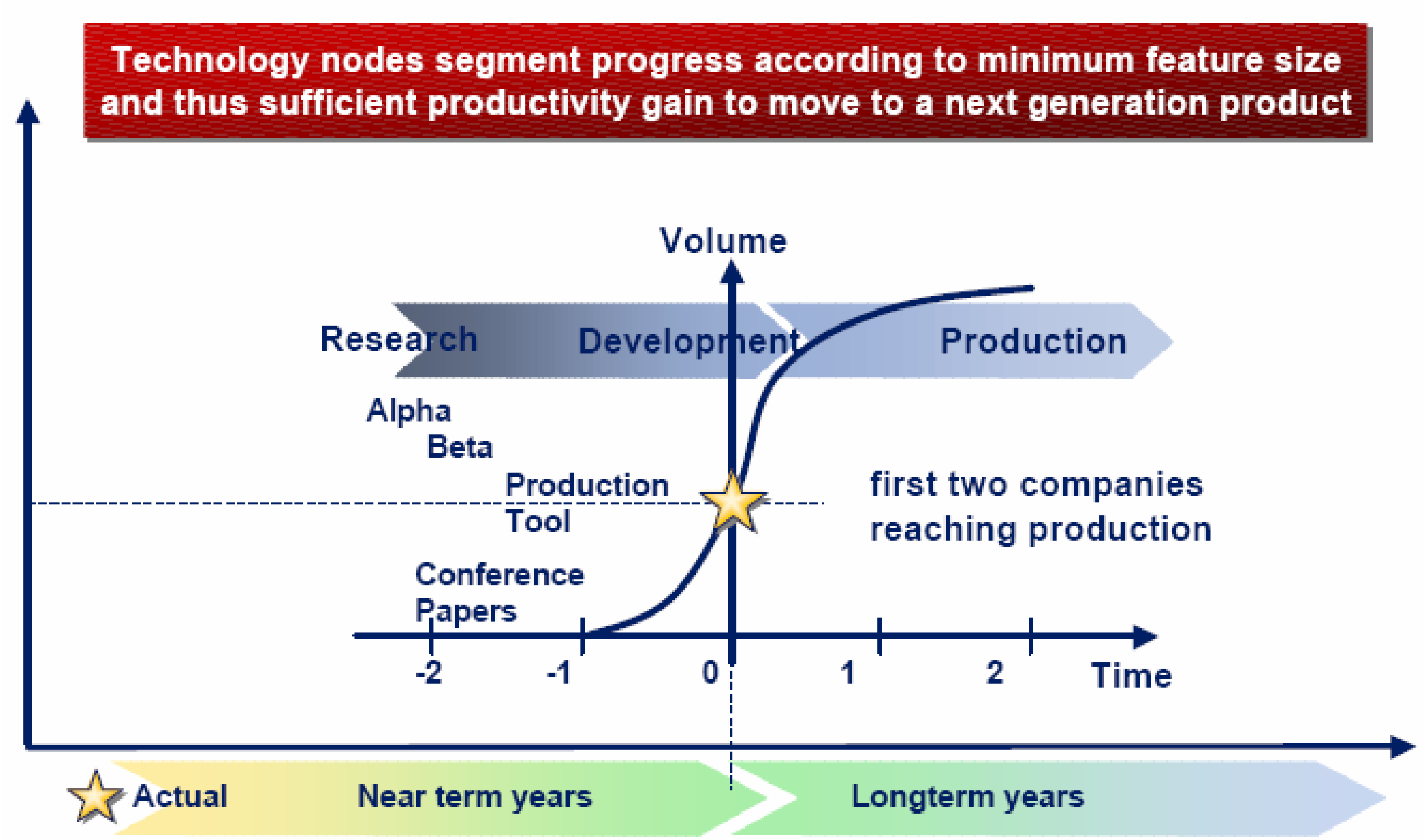
Heat becoming an unmanageable problem



Intel Developer Forum, Spring 2004 - Pat Gelsinger

The need for device modeling

1. Increased costs for R&D and production facilities, which are becoming too large for any one company or country to accept.
2. Shorter process technology life cycles.
3. Emphasis on faster characterization of manufacturing processes, assisted by modeling and simulation.



With permission from Intel Corp.

Why TCAD?

TCAD: Technology for Computer Aided Design

- Evaluating "what-if" scenarios rapidly
- Providing problem diagnostics
- Providing full-field, in-depth understanding
- Providing insight into extremely complex problems/phenomena/product sets
- Decreasing design cycle time (savings on hardware build lead-time, gain insight for next product/process)

1. Shortening time to market

Some TCAD Prerequisites Are:

- Modeling and simulation require enormous technical depth and expertise not only in simulation techniques and tools but also in the fields of physics and chemistry.
- Laboratory infrastructure and experimental expertise are essential for both model verification and input parameter evaluations in order to have truly effective and predictive simulations.
- Software and tool vendors need to be closely tied to development activities in the research and development laboratories.

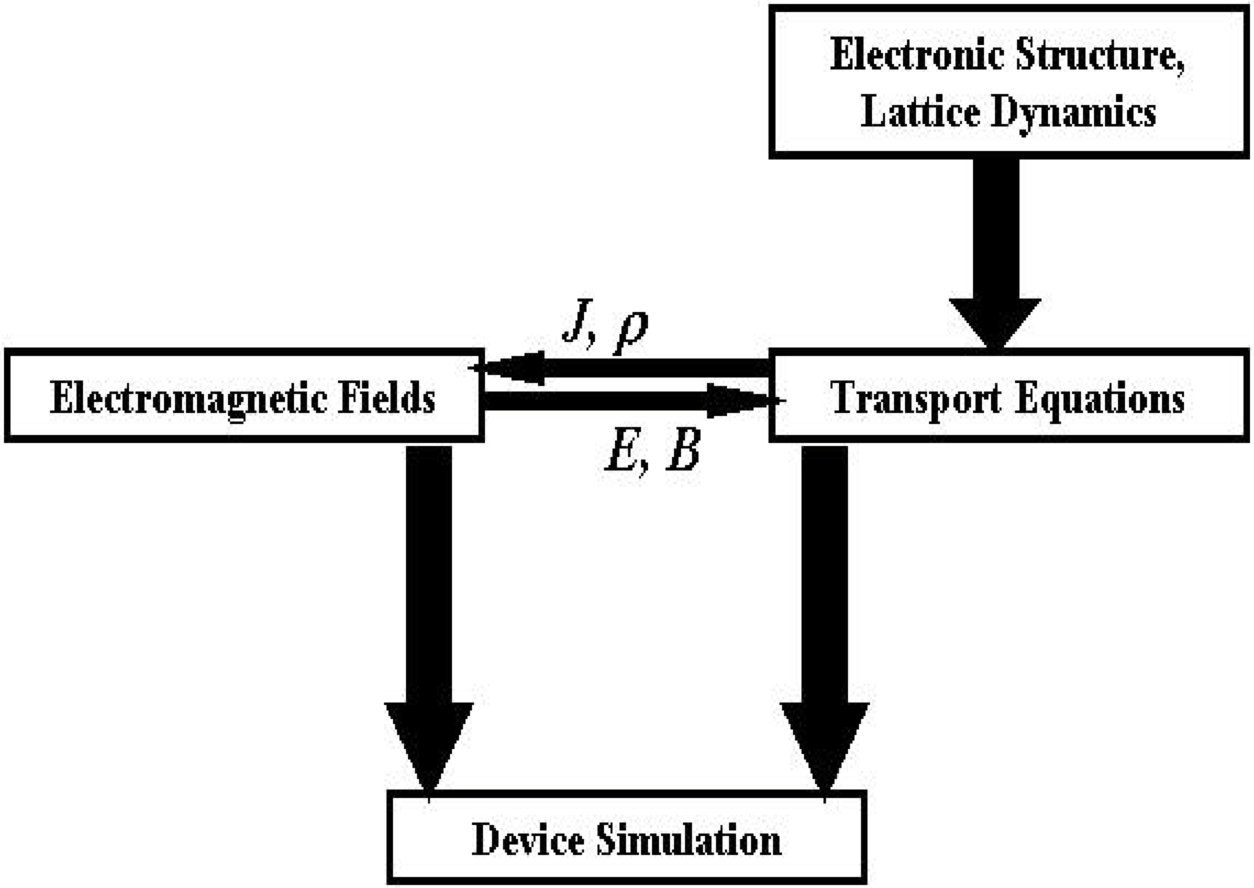
R. Dutton, Stanford University, the father of TCAD.

Historical Development of Device Simulation:

- **1964:** Gummel introduced the decoupled scheme for the solution of the Poisson and the continuity equations for a BJT
- **1968:** de Mari introduced the scaling of variables that is used even today and prevents effectively overflows and underflows
- **1969:** Sharfetter and Gummel, in their seminal paper that describes the simulation of a 1D Silicon Read (IMPATT) diode, introduced the so-called Sharfetter-Gummel discretization of the continuity equation

H. K. Gummel, "A self-consistent iterative scheme for one-dimensional steady state transistor calculation", *IEEE Transactions on Electron Devices*, Vol. 11, pp.455-465 (1964).
A**. DeMari**, "An accurate numerical steady state one-dimensional solution of the p-n junction", *Solid-state Electronics*, Vol. 11, pp. 33-59 (1968).
D. L. Scharfetter and D. L. Gummel, "Large signal analysis of a Silicon Read diode oscillator", *IEEE Transaction on Electron Devices*, Vol. ED-16, pp.64-77 (1969).

Coupling of Transport Equations to Poisson and Band-Structure Solvers

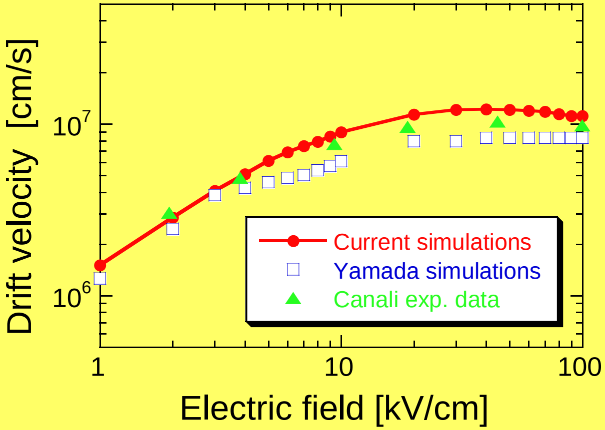


D. Vasileska and S.M. Goodnick, *Computational Electronics*, published by Morgan & Claypool , 2006.

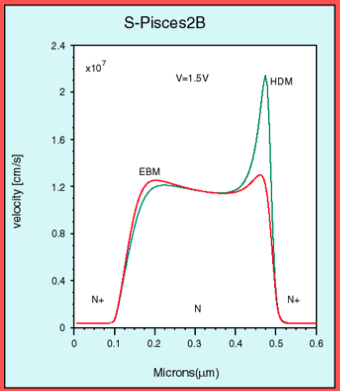
What Transport Models exist?

- Semiclassical **FLUID** models (ATLAS, Sentaurus, Padre)
  - »Drift – Diffusion
  - »Hydrodynamics

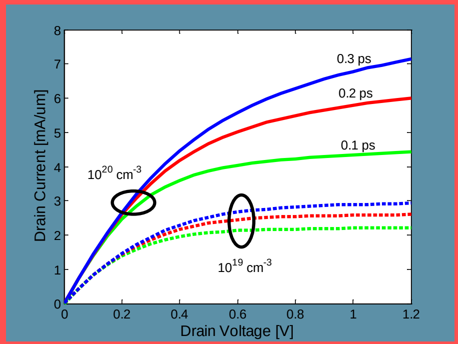
1. **PARTICLE DENSITY**
2. velocity saturation effect
3. mobility modeling crucial



1. Particle density
2. **DRIFT VELOCITY, ENERGY DENSITY**
3. velocity overshoot effect



problems



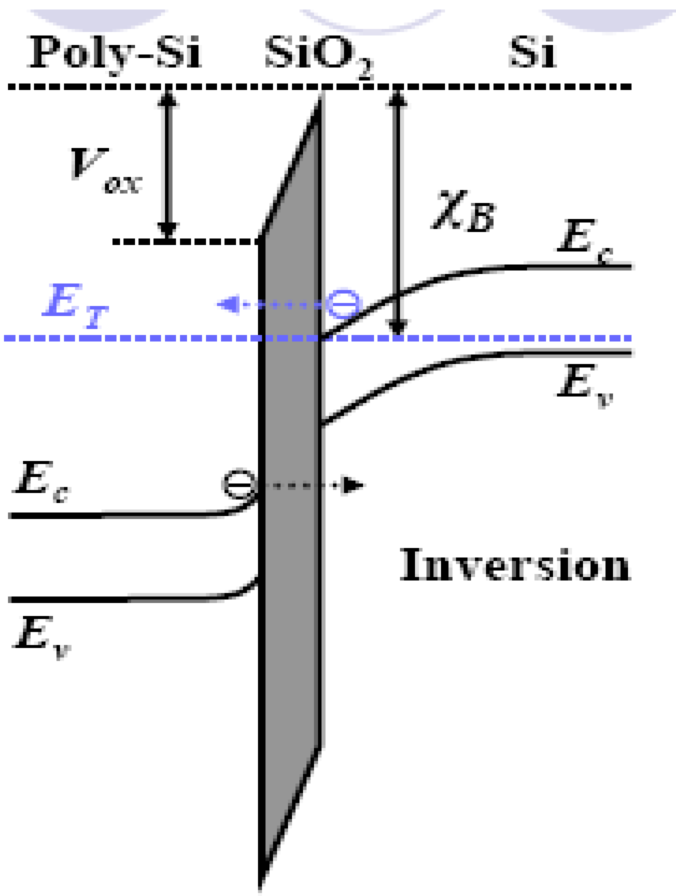
What Transport Models Exist?

- Semi-classical **PARTICLE-BASED** Models:
  - »Direct solution of the BTE Using Monte Carlo method

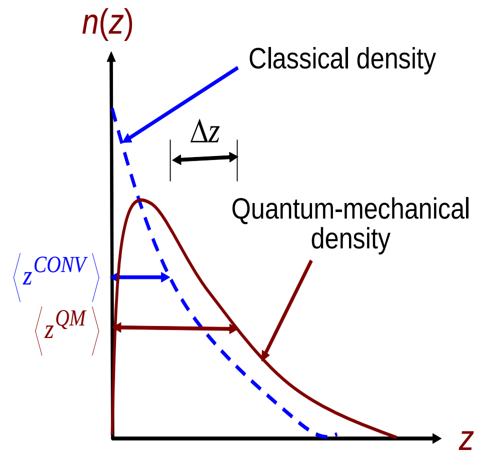
    - ✓ Eliminates the problem of Energy Relaxation Time Choice
    - ✓ Accurate up to semi-classical limits
    - ✓ One can describe scattering very well
    - ✓ Can treat ballistic transport in devices

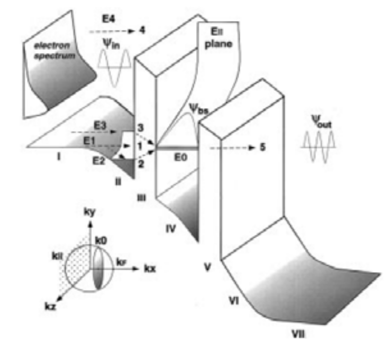
Why Quantum Transport?

1. Quantum Mechanical TUNNELING

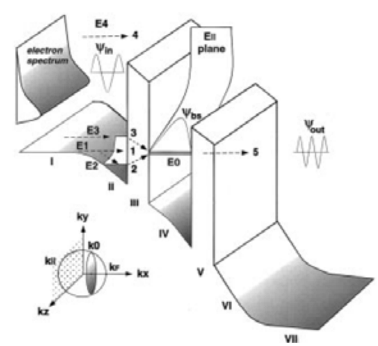


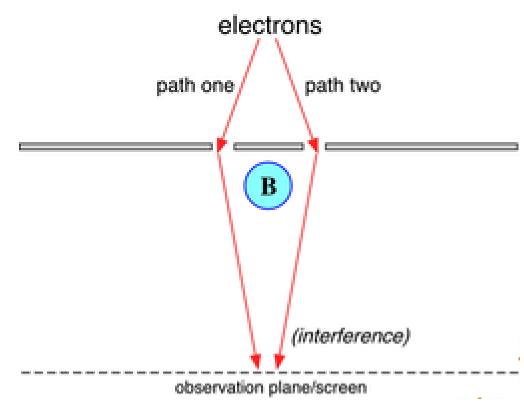
2. SIZE-QUANTIZATION





3. QUANTUM INTERFERNCE EFFECT





What Quantum Transport Models Exist?

- Quantum-mechanical **WIGNER** Function and **DENSITY** Matrix Methods:
  - »Can deal with correlations in space
  - »BUT NOT WITH CORRELATIONS IN TIME

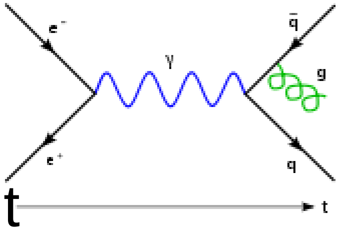
Advantages: Can treat SCATTERING

Disadvantages: LONG SIMULATION TIMES

What Transport Models Exist?

Non-Equilibrium Green's Functions (NEGF)

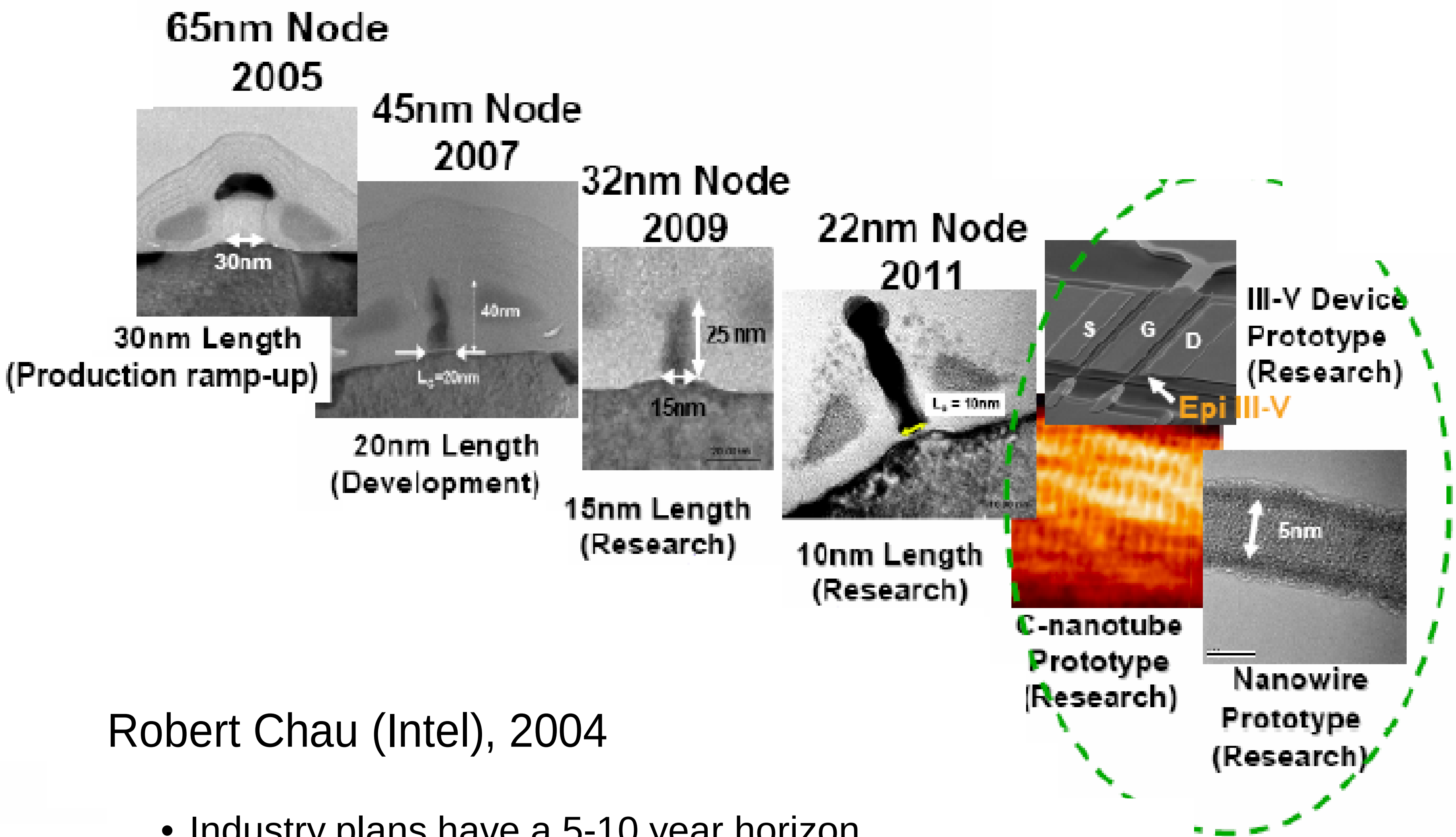
- MOST fundamental and accurate
- Considered by many to be the MOST difficult quantum approach
- FORMULATION OF SCATTERING rather straightforward and theoretically sound including incoherence and irreversibility
- IMPLEMENTATION OF SCATTERING rather difficult
- Computationally INTENSIVE



Length Scales and Interactions Determine the Most Appropriate Model

	$L << l_{e-ph}$			$L \sim l_{e-ph}$	$L >> l_{e-ph}$
	$L < \lambda$	$L < l_{e-e}$	$L >> l_{e-e}$		
Transport Regime	Quantum	Ballistic	Fluid	Fluid	Diffusive
Scattering	Rare	Rare	e-e (Many), e-ph (Few)		Many
Model:					
Drift-Diffusion					
Hydrodynamic	Quantum Hydrodynamic				
Monte Carlo					
Schrodinger/Green's Functions	Wave				
Applications	Nanowires, Superlattices	Ballistic Transistor	Current IC's	Current IC's	Older IC's

Technical Developments to enable Moore's Law



Robert Chau (Intel), 2004

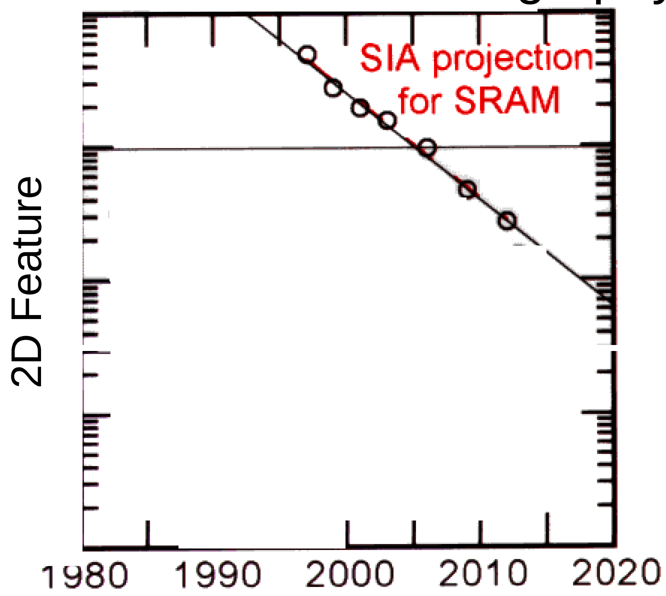
- Industry plans have a 5-10 year horizon
- Industry has been on time:
  - 32nm node predicted in 2004 and announced 2009
- **There are NO technically viable solutions beyond 2015**

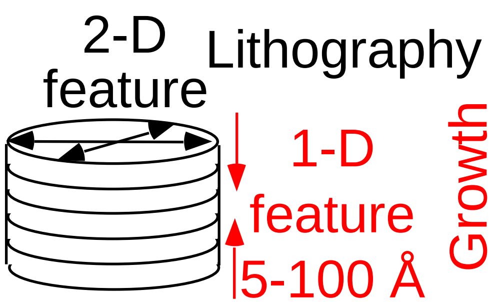
A Second Look at Moore's Law
Shrinking Device Sizes

Exponential performance increase:

- Enabled by
  - **device miniaturization**
  - chip size increase
- Limited by:
  - Costs of fabrication

Moore's Law for Lithography

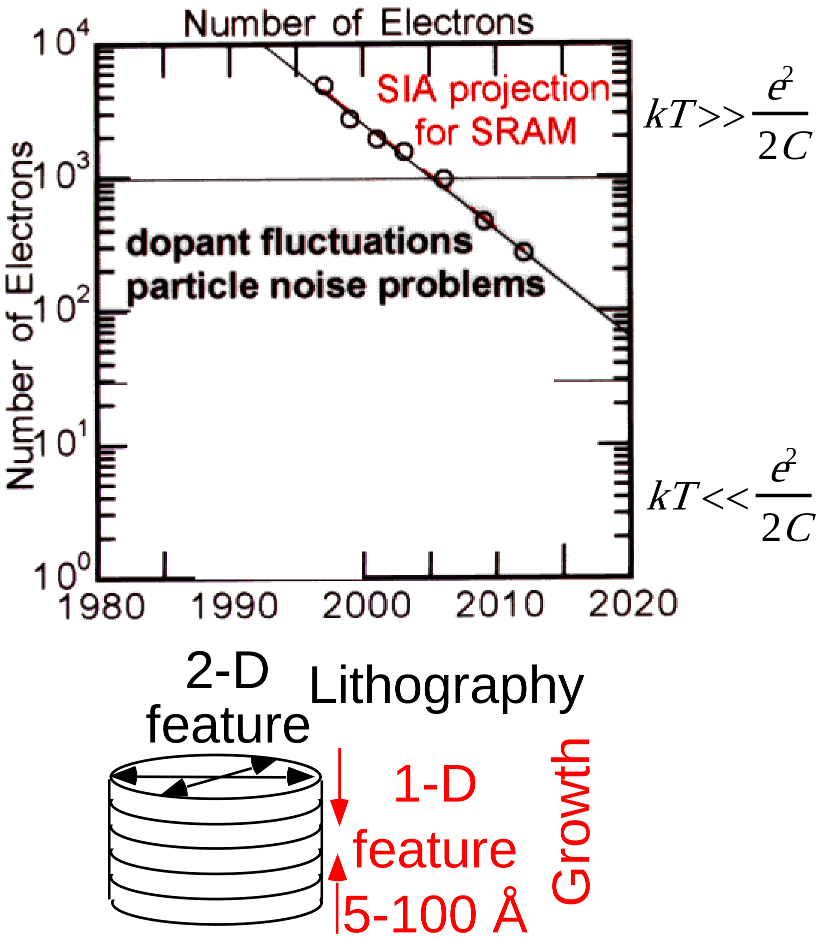




A Third Look at Moore's Law
Countable number of electrons

Exponential performance increase:

- Enabled by
    - **device miniaturization**
    - chip size increase
- Limited by:
    - Costs of fabrication
    - **Discrete atoms/electrons**



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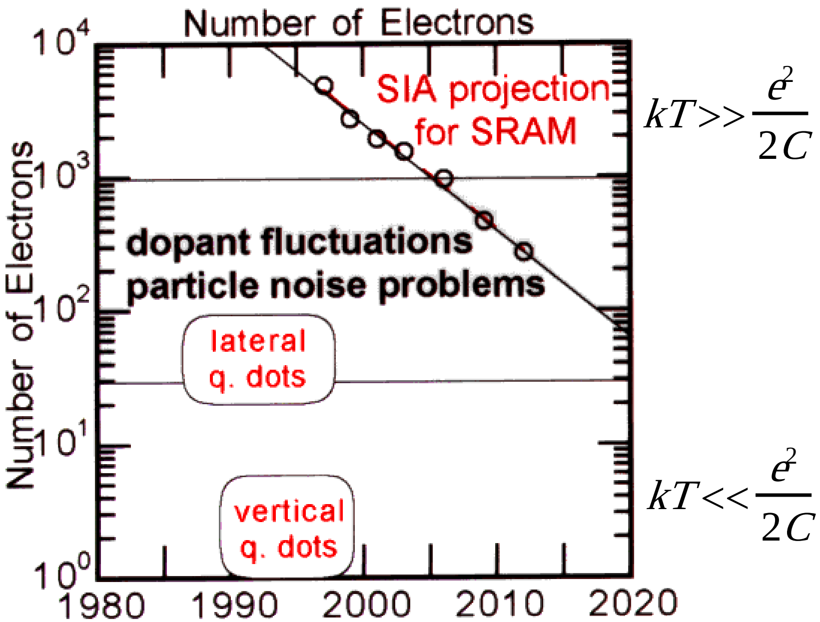
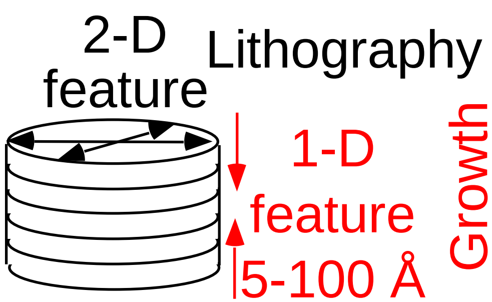


Quantum Dots

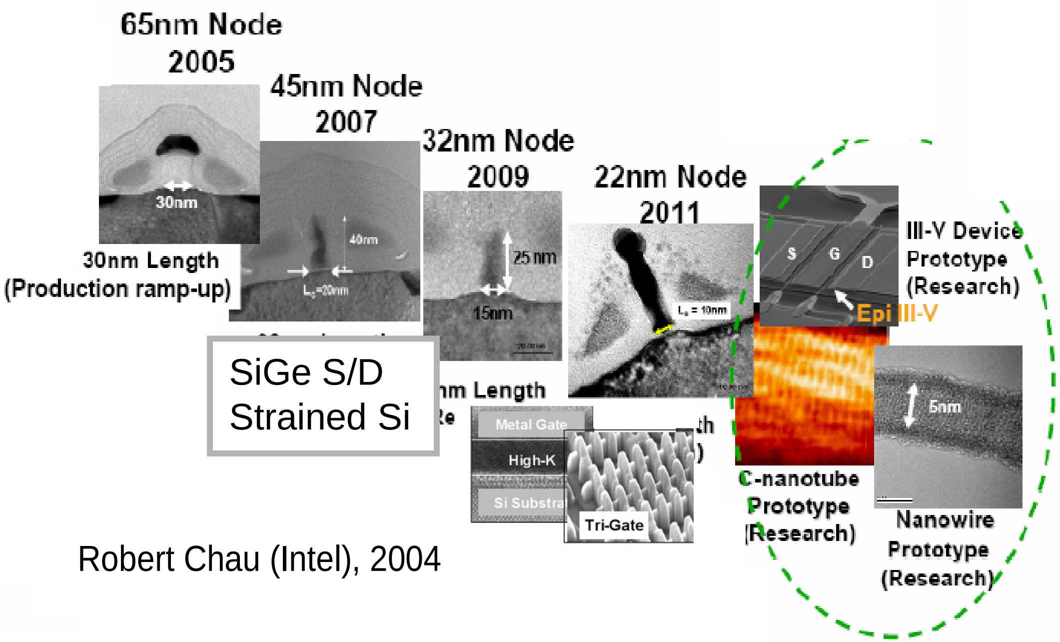
- Artificial Atoms - Electron Boxes

1D Heterostructures

- Lasers and detectors
- Fast electronic devices



Device Trends and Challenges



Robert Chau (Intel), 2004

Observations:

- 3D spatial variations on nm scale
- Potential variations on nm scale
- New channel materials (Ge, III-V)

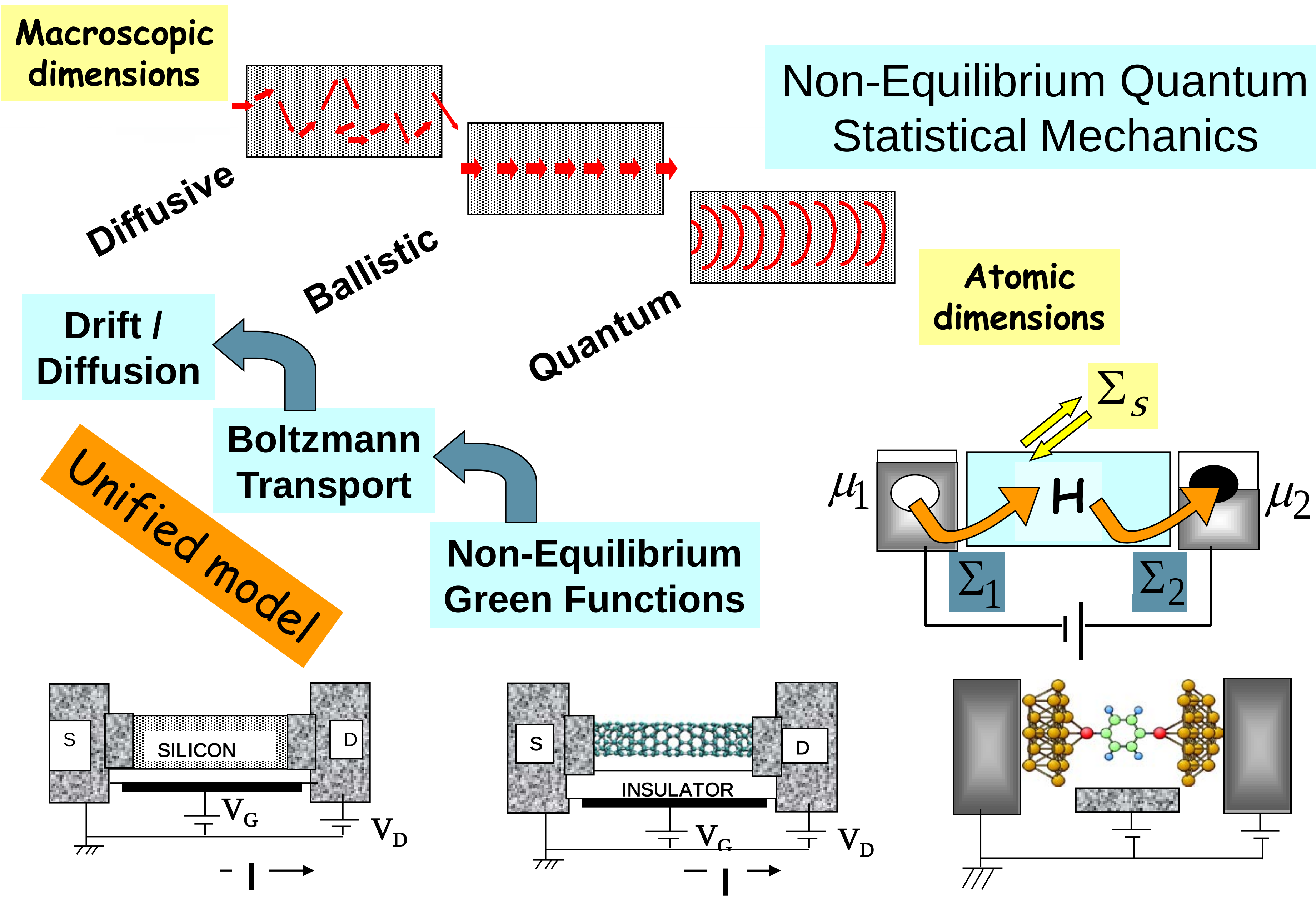
Questions / Challenges

- Strain ?
- Quantization?
- Crystal orientation?
- Atoms are countable; does granularity matter? Disorder?
- New material or new device?

Assertions of importance

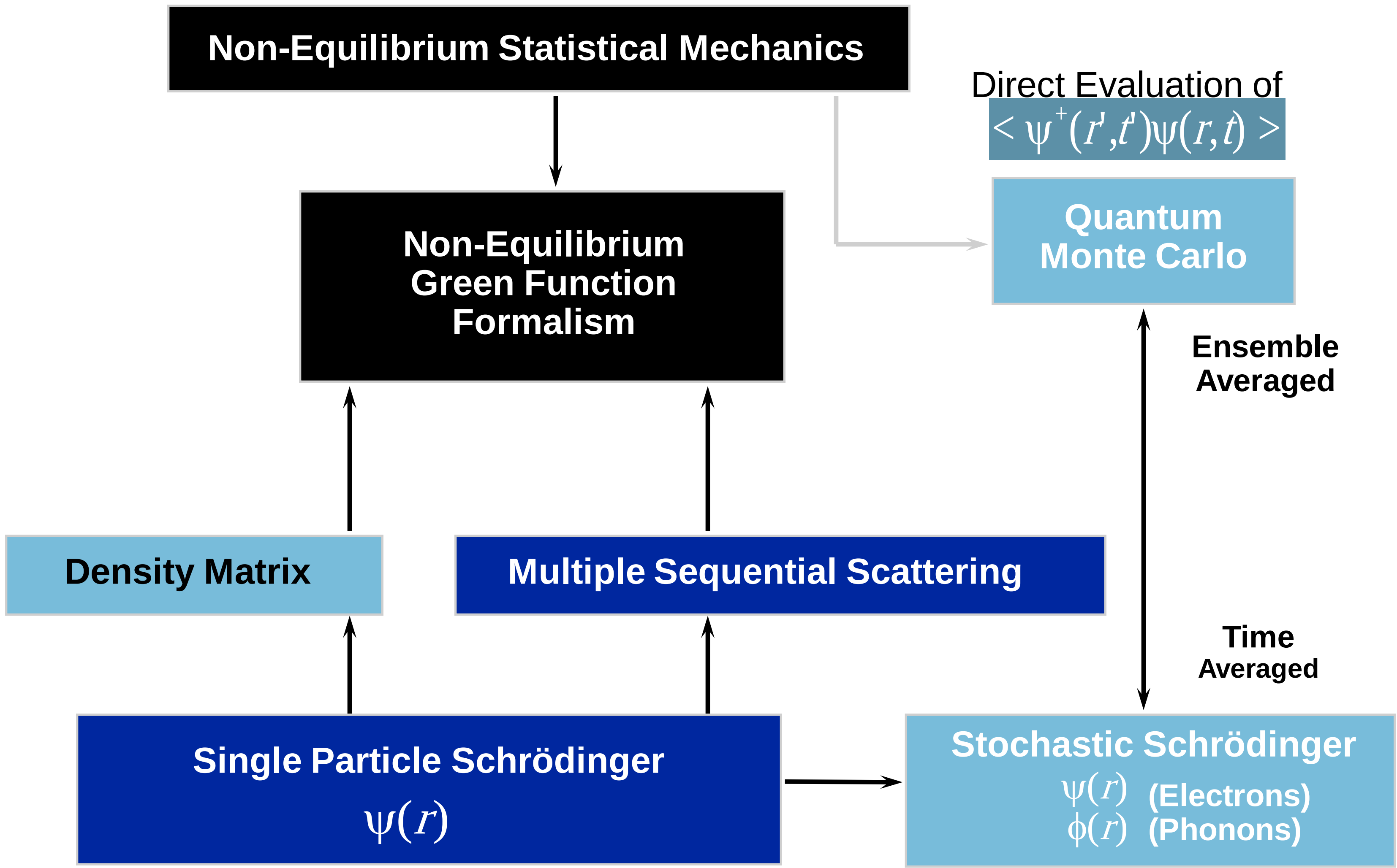
- High bias / non-equilibrium
- Quantum mechanics
- Atomistic representation
  - » Band coupling, non-parabolicity, valley splitting
  - » Local (dis)order, strain and orientation

Quantum Transport far from Equilibrium

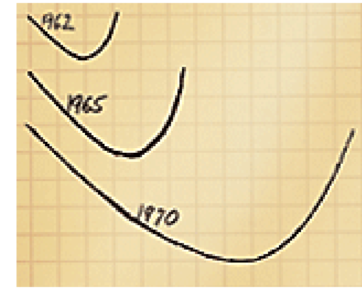


Available and Explored Theories

- The non-equilibrium Green function formalism underlies NEMO.
- All of the approaches shown were considered.
- Approaches in light blue were dropped. Approaches in dark blue were incorporated.



Semiconductor Industry has Fundamental Issues and Problems



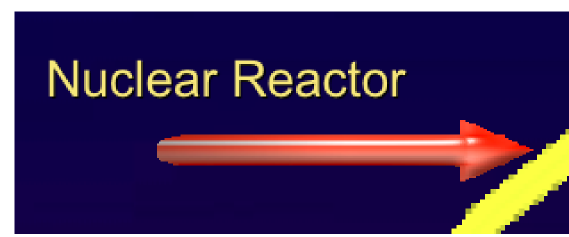
- Driven by a revenue stream –
  => it must be cheaper and better
  => so people throw away their old computers

- Devices are at the nanometer scale
  => wavelength of the electrons
  !!! Existing tools are not fundamentally quantum mechanics based

- Devices now consist of "countable number of atoms
  => does the atomistic granularity matter?
  !!! Existing tools are based on continuum matter theory

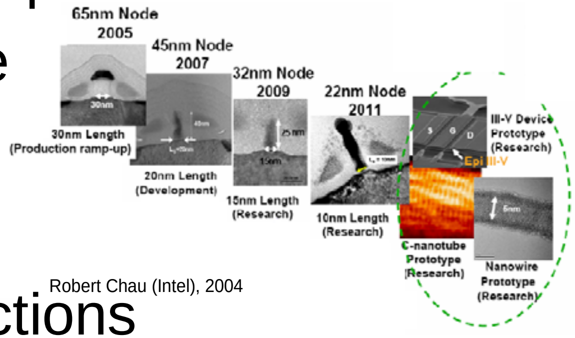
- Devices consume too much heat
  => need alternative designs?
  !!! Existing tools cannot handle
  QM, atomistic granularity, and thermal transport

NEMO / OMEN



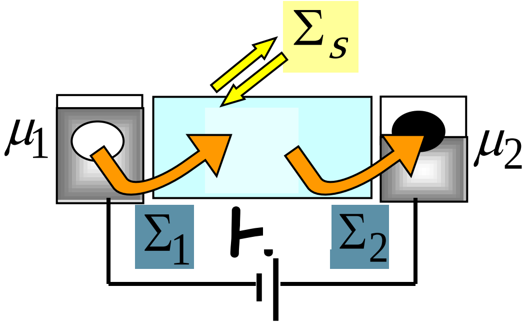
Nanoelectronic Modeling – NEMO Assertions and Agenda

- Production level, industrial semiconductor devices:
  - »Show spatial arrangements in 3D – no longer planar
  - »Have dimensions where atoms are countable
  - »Involve new materials



Robert Chau (Intel), 2004

- Fundamental theory for modeling
  - »Needs to include high bias and carrier interactions
  - »Needs to be on an atomistic basis
  - »Has been developed: NEGF-Non-Equilibrium Green Functions
- Model implementations:
  - »Must be validated against experimental data
  - »Predictive
  - »Deliver physical insight
  - »Computationally efficient



- **Must be taught to the next generation engineers!**