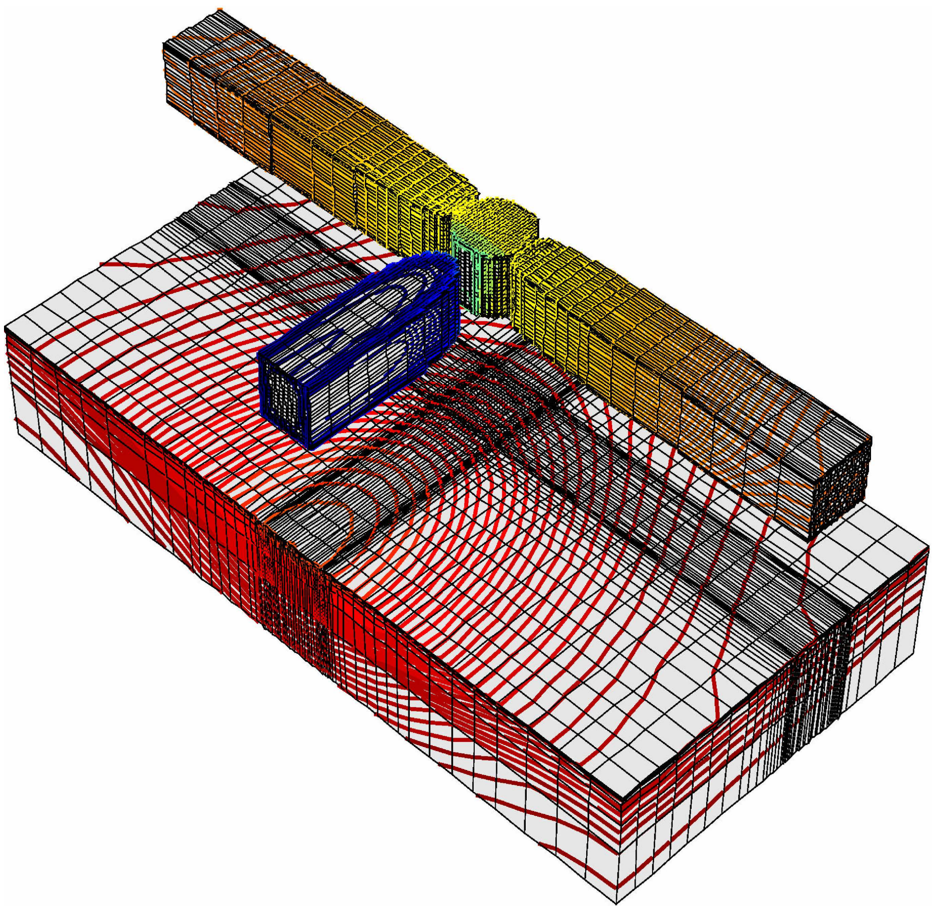
Quantum transport effects and their modeling



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SNDT Taiwan, May 2004

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Outline

- ★ Motivation
- ★ Overview: Simulation models
- ★ “Conventional” device simulation
- ★ Classical Monte-Carlo simulation
  - – Treatment of non-localities
  - – Strained silicon devices
- ★ Modeling of quantum effects
- ★ Conclusion

Motivation

★ Scaling is the driving force behind the semiconductor revolution

Year	1999	2002	2005	2008	2011	2014
Technology node (nm)	180	130	100	70	50	35

Physical gate length: 9 nm

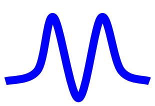
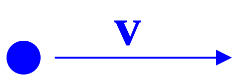
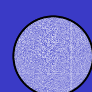
★ Reduced device dimensions require refined simulation models:

– higher fields ⇨ non–local transport effects

– quantum mechanics

G.E.Moore, *Electronics*, **38**(8) (1965); M.Lundstrom, *Science* **299**, 210 (2003)

A Taxonomy of Simulation Models

	near equilibrium dissipative (local mobility)	quasi–ballistic	fully ballistic
quantum mechanics  $-\frac{\hbar^2}{2m^*}\nabla^2$	Quantum drift–diffusion	NEGF with Büttiker probes Wigner eq$^{\underline{n}}$	NEGF without $\Sigma_{scatter}$ Scattering matrix
classical mechanics 	Drift–diffusion  Hydro	Boltzmann eq$^{\underline{n}}$ (full band MC)	scattering free Boltzmann (analytic)

The Boltzmann Transport Equation (BTE)

$$\left(\frac{\partial}{\partial t} + \mathbf{v}(\mathbf{k}) \cdot \boldsymbol{\nabla}_{\mathbf{r}} - \frac{e}{\hbar}\mathbf{E}(\mathbf{r}) \cdot \boldsymbol{\nabla}_{\mathbf{k}}\right) f(\mathbf{r}, \mathbf{k}, t) = \left(\frac{\mathrm{d}f}{\mathrm{d}t}\right)_{\mathrm{coll}}$$

★ Device simulation is based on the kinetic theory of gases.

★ Dynamic variable: Classical distribution function

$$f(\mathbf{r}, \mathbf{k}, t)\, \mathrm{d}^3 r\, \mathrm{d}^3 k = \#(\text{particles in } \mathrm{d}^3 r\, \mathrm{d}^3 k)$$

The “Conventional” Simulation Models

★ BTE: integro–differential eq$^{\underline{n}}$ over $\mathbb{R}^7$.

$\Rightarrow$ Numerical effort rather high.

★ Reduce effort by the Method of Moments

- New dynamic variables:
  $\mathbf{k}$–averages of $\otimes^n \mathbf{v}(\mathbf{k})\, f(\mathbf{r}, \mathbf{k}, t)$
- Use only the (two) lowest moments.
- Introduce a local parameterization of μ.

$\Rightarrow$ Hydrodynamic eq$^{\underline{n}}$s / Drift–Diffusion eq$^{\underline{n}}$s

Limitations of the “Conventional” Models

★ Assumptions

– local thermal equilibrium

– $\mathbf{v}_{\mathrm{mean}}$ is a function of local quantities.

✘ fail in very small devices:

✘ not enough scattering for local thermalization

✘ ballistic contributions to $\mathbf{v}_{\mathrm{mean}}$ —
electron velocity depends on the history
$\Rightarrow$ velocity overshoot.

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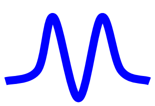
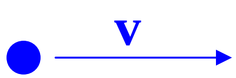
quantum mechanics  $-\frac{\hbar^2}{2m^*}\nabla^2$	Quantum drift–diffusion	NEGF with Büttiker probes Wigner eq<u>n</u>	NEGF without $\Sigma_{scatter}$ Scattering matrix
classical mechanics 	Drift–diffusion Hydro	Boltzmann eq<u>n</u> (full band MC)	scattering free Boltzmann (analytic)

Direct Solution of the Boltzmann equation

★ Characteristics of the Boltzmann equation:
- High dimensionality of the space of possible f,
- Stochastic nature of the scattering term.

✗ Direct discretization problematic / inefficient.

✓ Monte–Carlo methods well suited.

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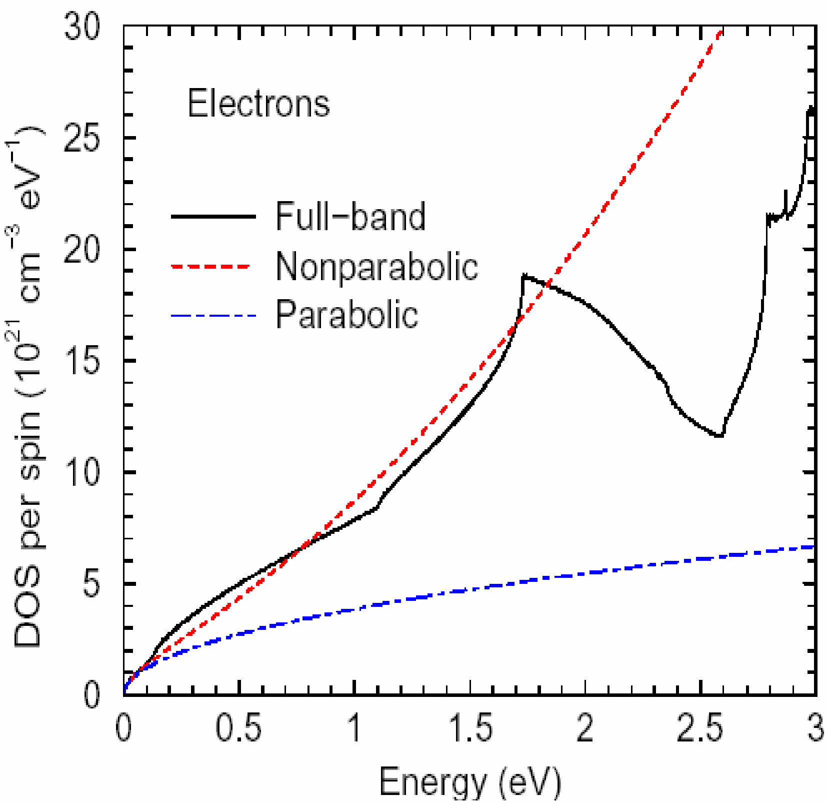
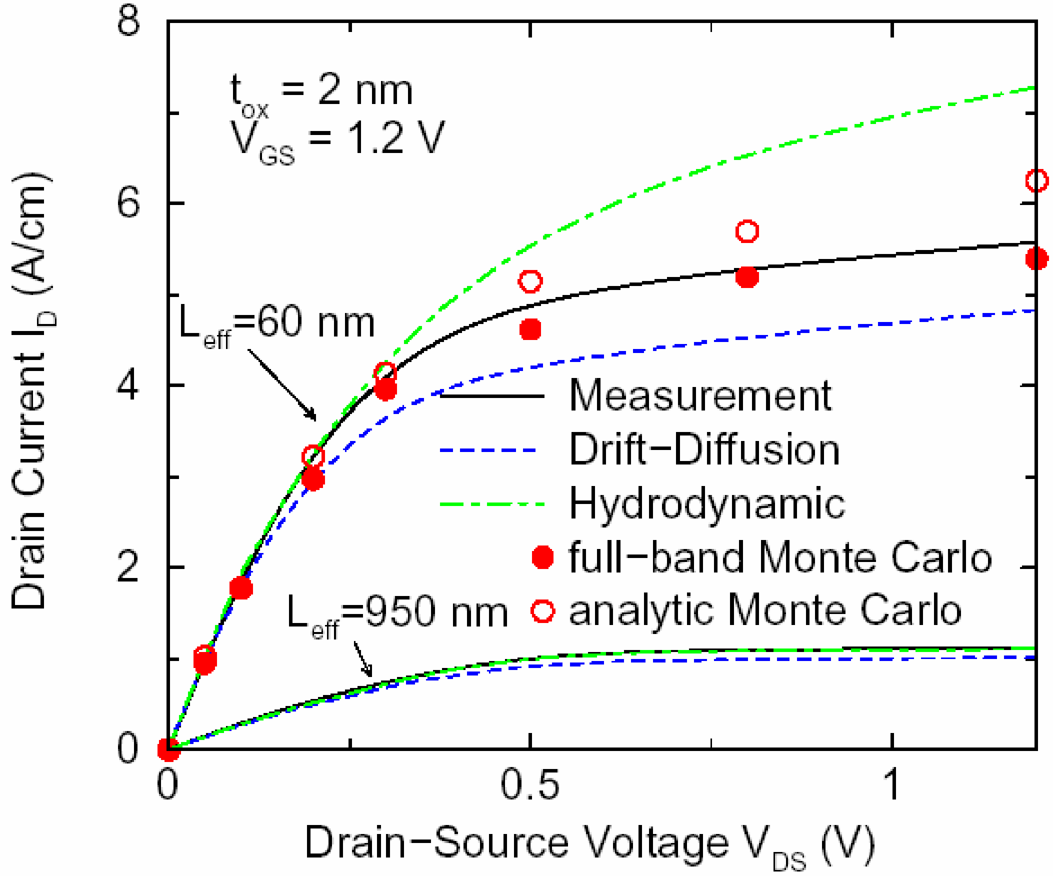
Density–of–States DOS



$$\mathcal{D}(\epsilon) = \frac{1}{(2\pi)^3} \int_{\epsilon(\mathbf{k})=\epsilon} \frac{\mathrm{d}F}{|\nabla_{\mathbf{k}}\epsilon(\mathbf{k})|} = \frac{1}{(2\pi)^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \sqrt{\epsilon}$$

$\rightarrow$ phonon scattering rate (isotropic and parabolic)

Output Characteristics



Different simulation models

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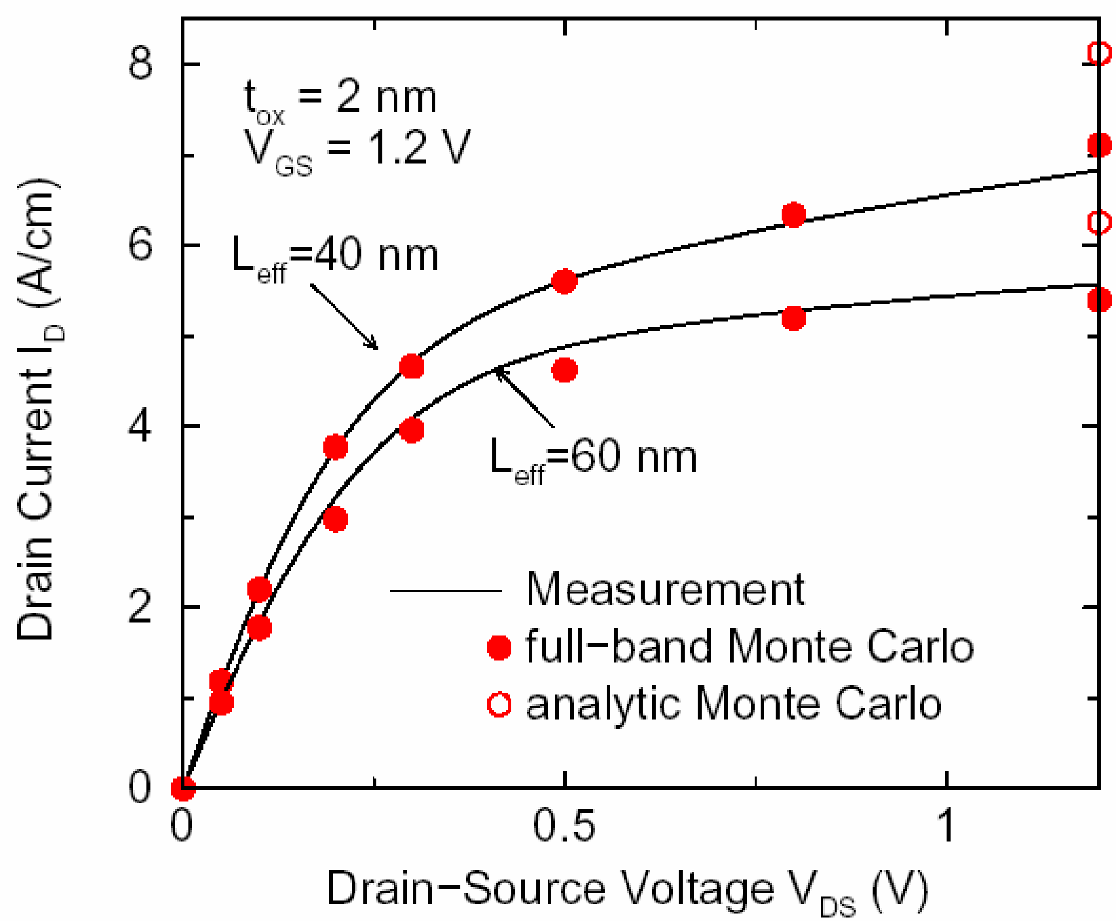
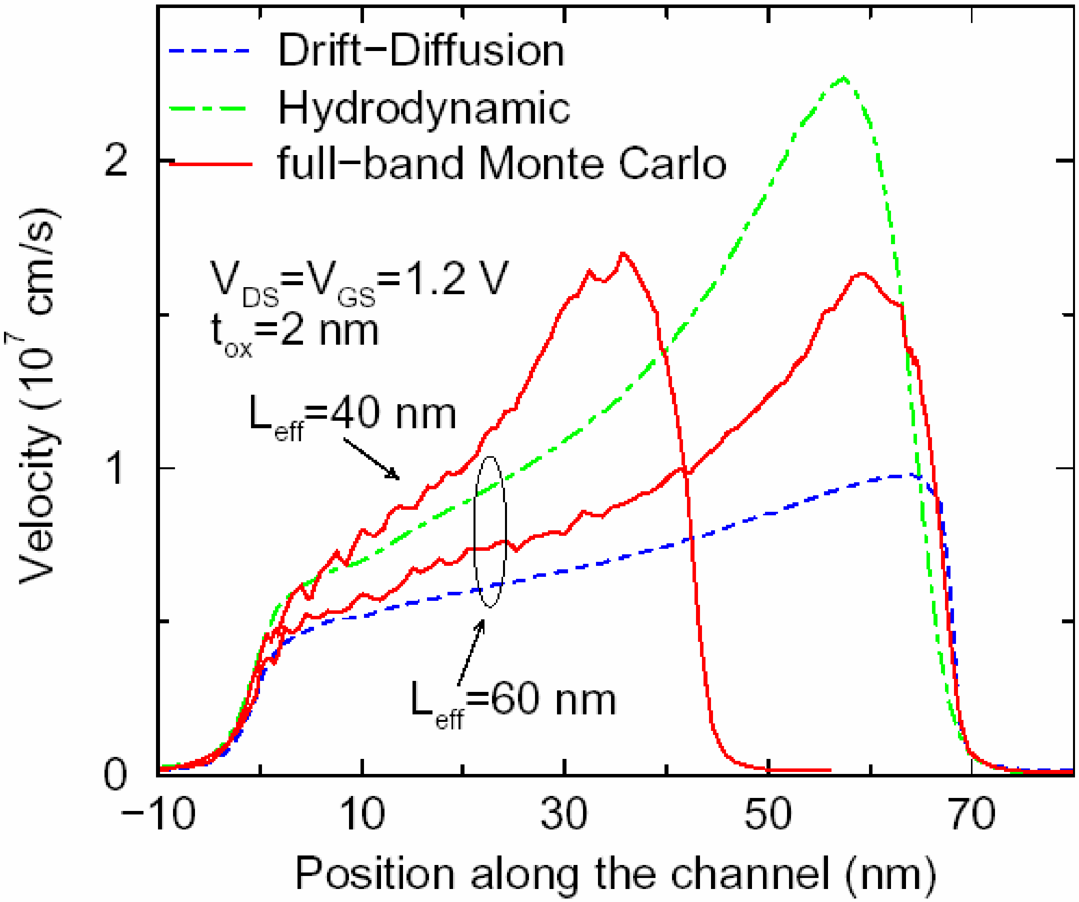
Output Characteristics



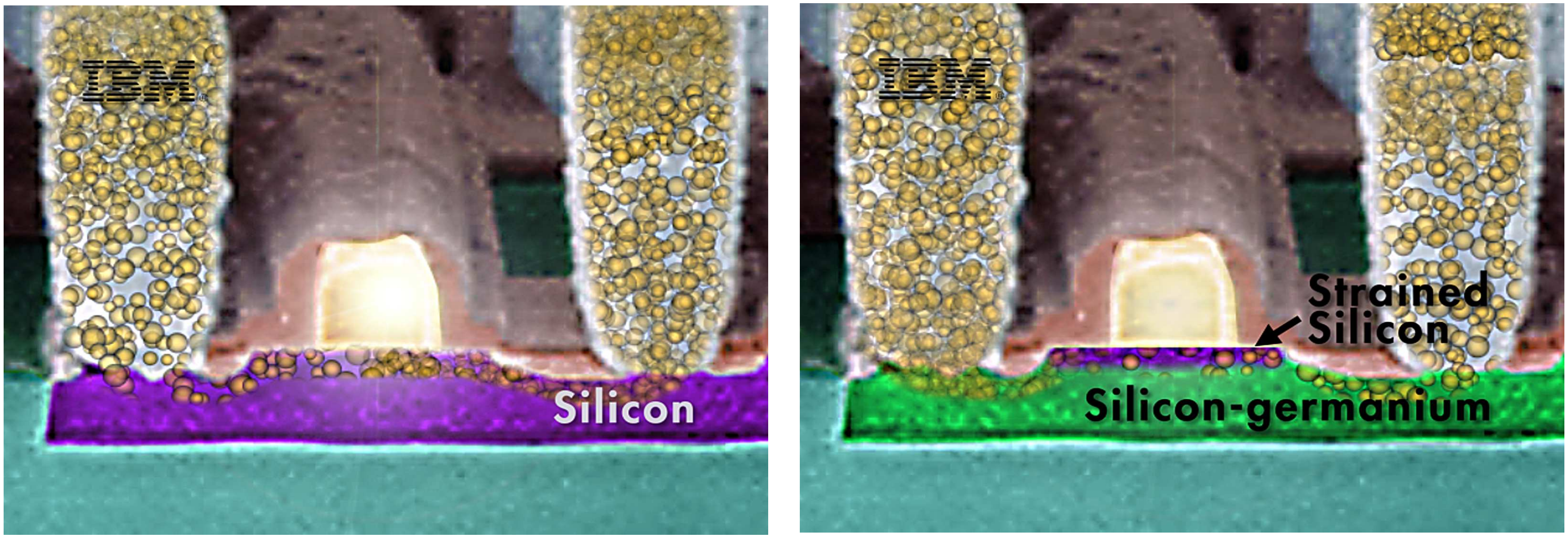
Different gate lengths

Velocity Profiles along the Channel



Velocity in source–side of channel determines on–current

Strained Silicon

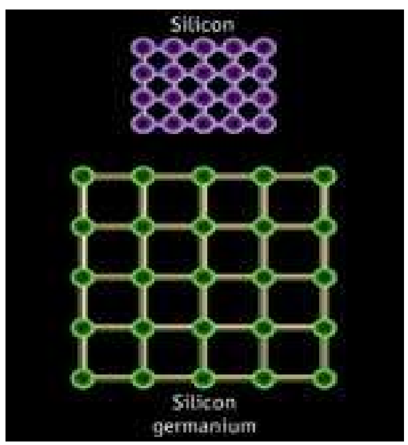


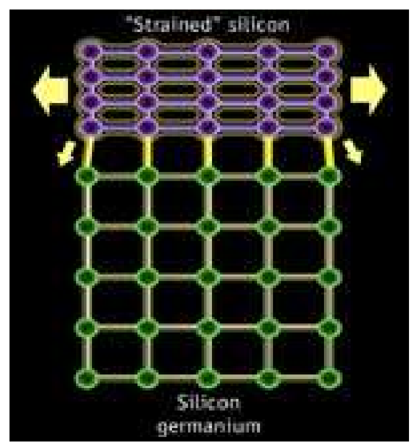
Silicon–Germanium and strained Silicon are now heavily used in semiconductor industry

★compute the mobility by bulk Monte–Carlo [input: band-structure of strained Si]

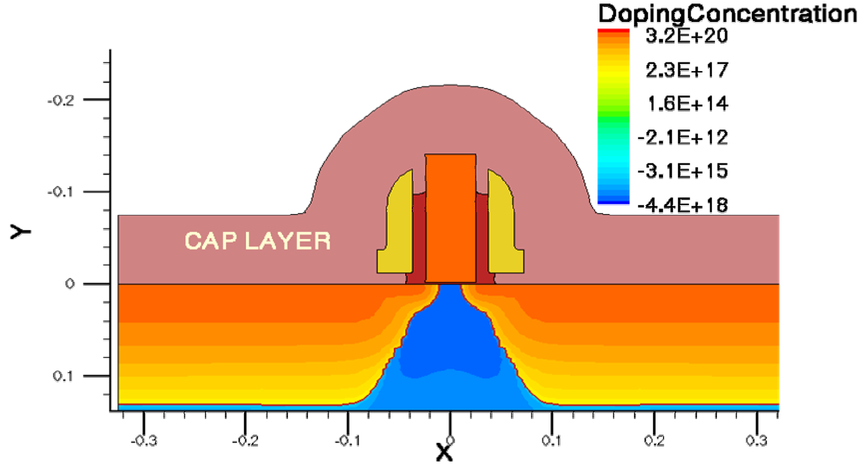
SiGe and strained Si Lattice constant

- ★ Silicon: 5.43 Å
- ★ Germanium: 5.66 Å
- ★ $Si_{1-x}Ge_x$: depends on the mole-fraction x.
- ★ Lattices of deposited layer will naturally adapt:
  - – SiGe on top of Silicon is under compressive stress
  - – Silicon on top of SiGe is stretched
  - – *increased mobility !!!*





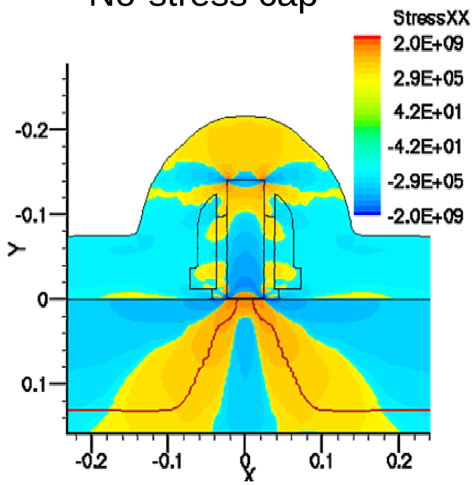
Strained CMOS – Strain in the Cap Layer

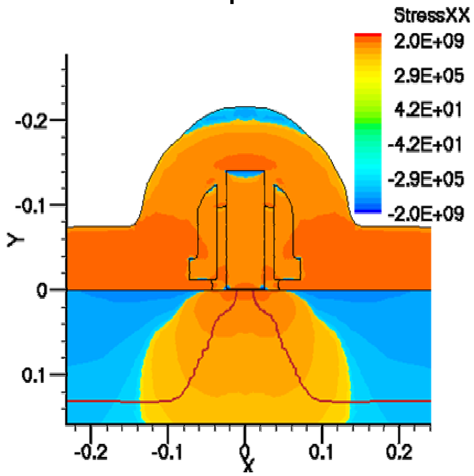


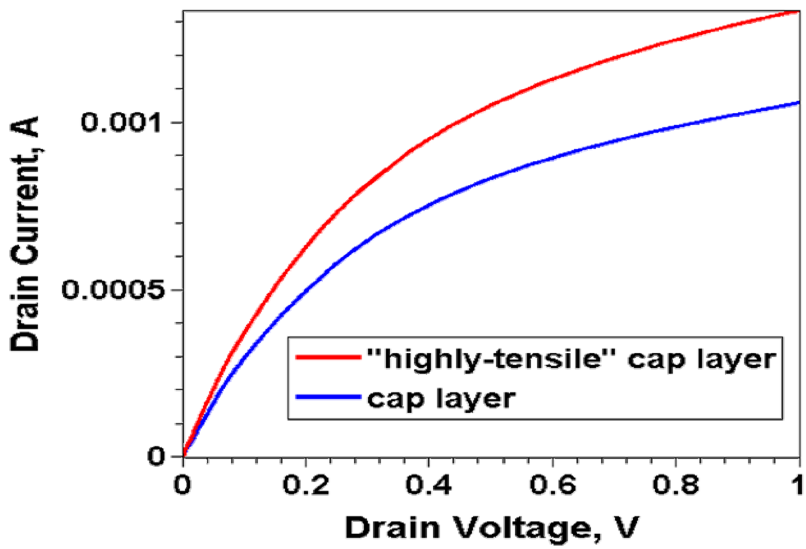
High tensile stress in the cap layer results in compressive stress in source and drain and tensile stress in the channel.

No-stress cap

stressed cap







The NMOS with the highly tensile stress cap layer shows an improved saturation current (approx. 14%).

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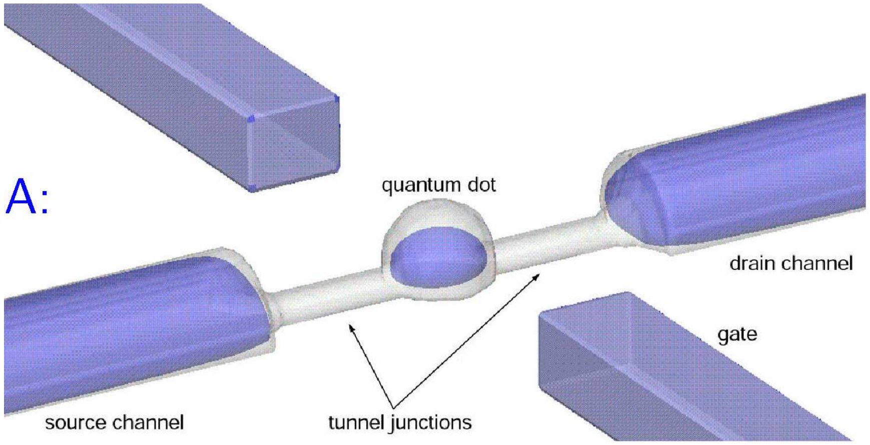
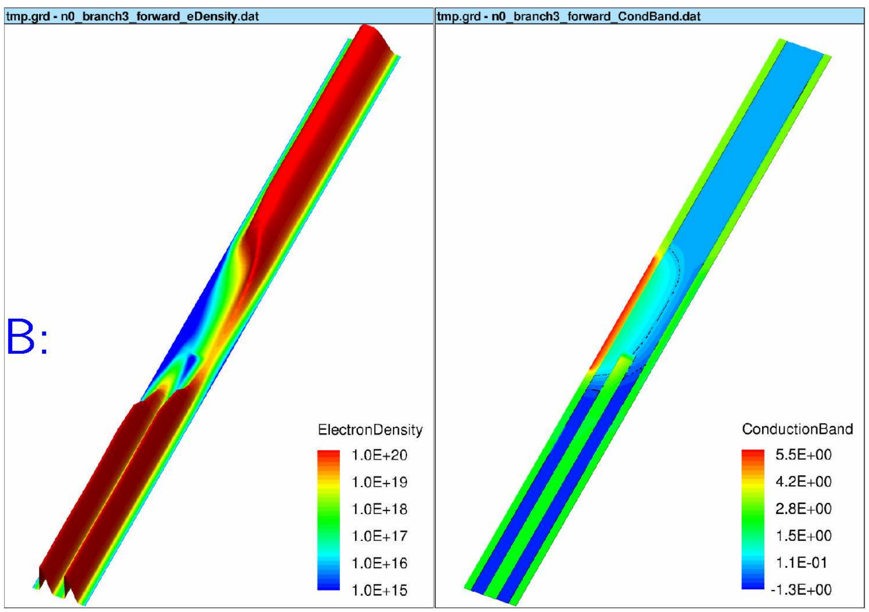
Quantum mechanics becomes important!

A:

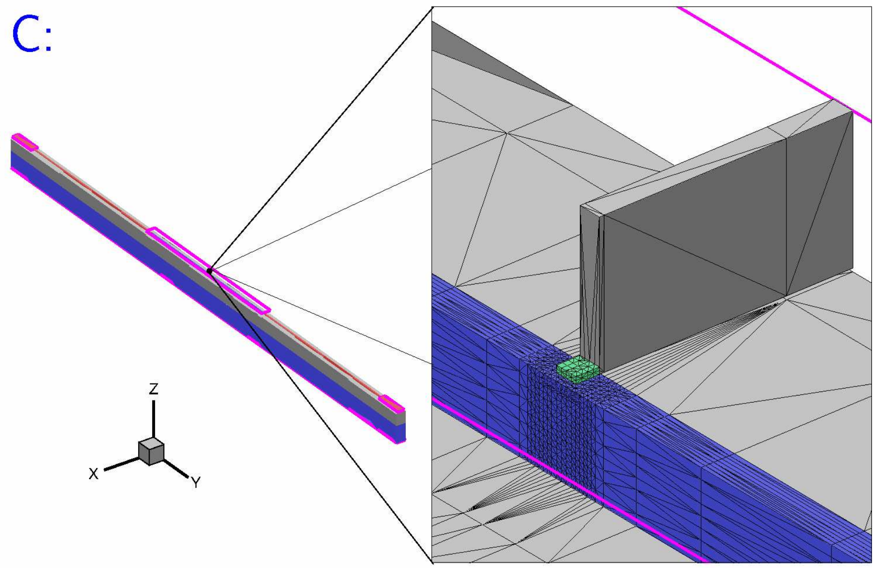


Nanodevices have
“critical dimensions”
comparable with the
electron wavelength.

B:

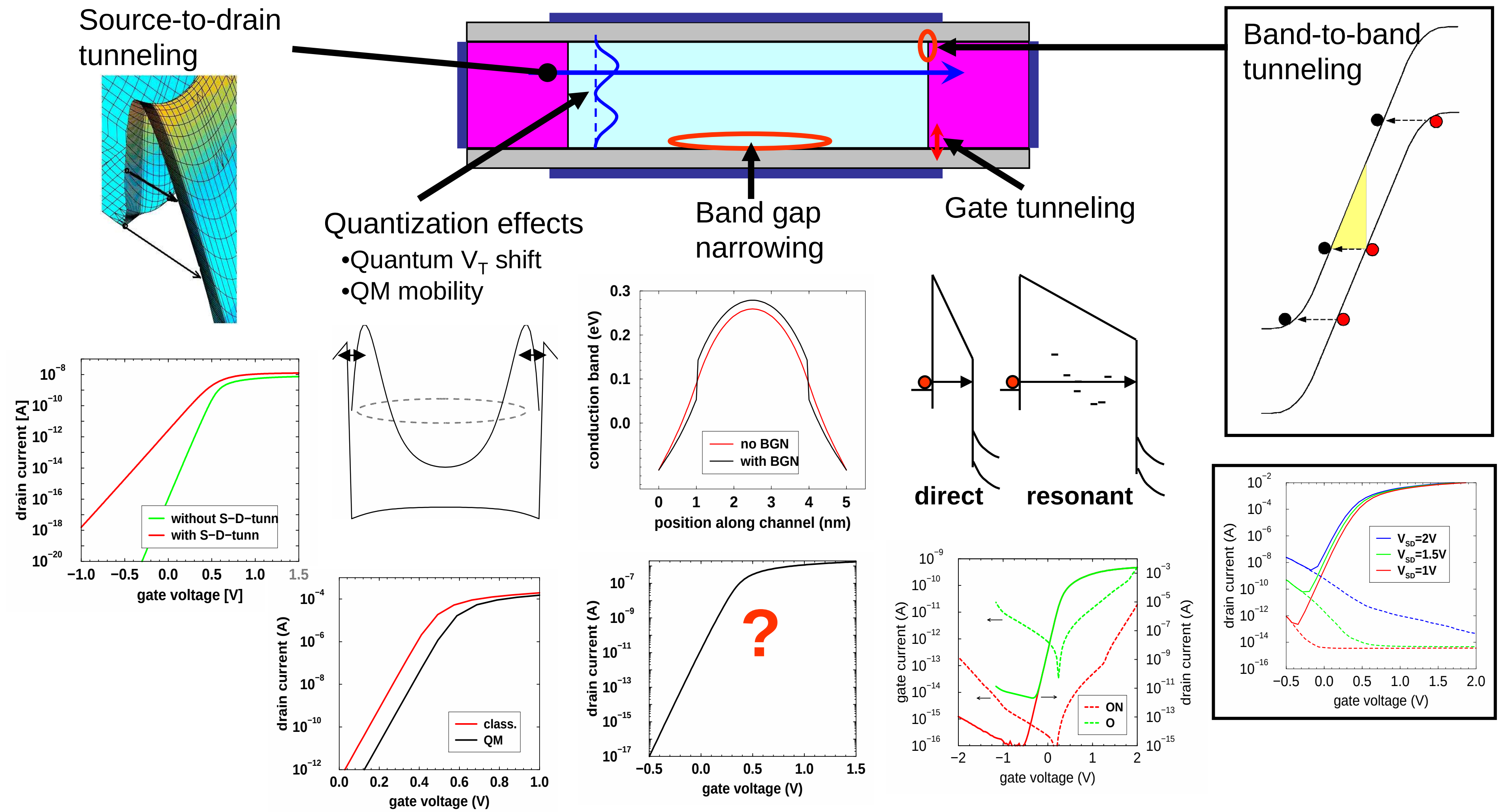


C:



A: Single electron transistors
B: Quantum–ballistic devices
C: QD flash memory

Five quantum effects



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classical mechanics $\mathbf{v}$	Drift–diffusion Hydro	Boltzmann eq$^{\underline{n}}$ (full band MC)	scattering free Boltzmann (analytic)

Quantum Ballistic Transport

- $\star$ Coherent transport
  - $\nexists$ inelastic scattering.
  - An e^- remains in a fixed Ψ (solution of Schrödinger eq$\underline{^n}$).
  - When occupied, Ψ carries a current $I(\Psi) \propto$ transmission probability $T(\epsilon)$.

- $\star$ Thermal carrier injection at the contacts.

$\Rightarrow$ Landauer–Büttiker formula:

from open boundary Schrödinger eq$\underline{^n}$

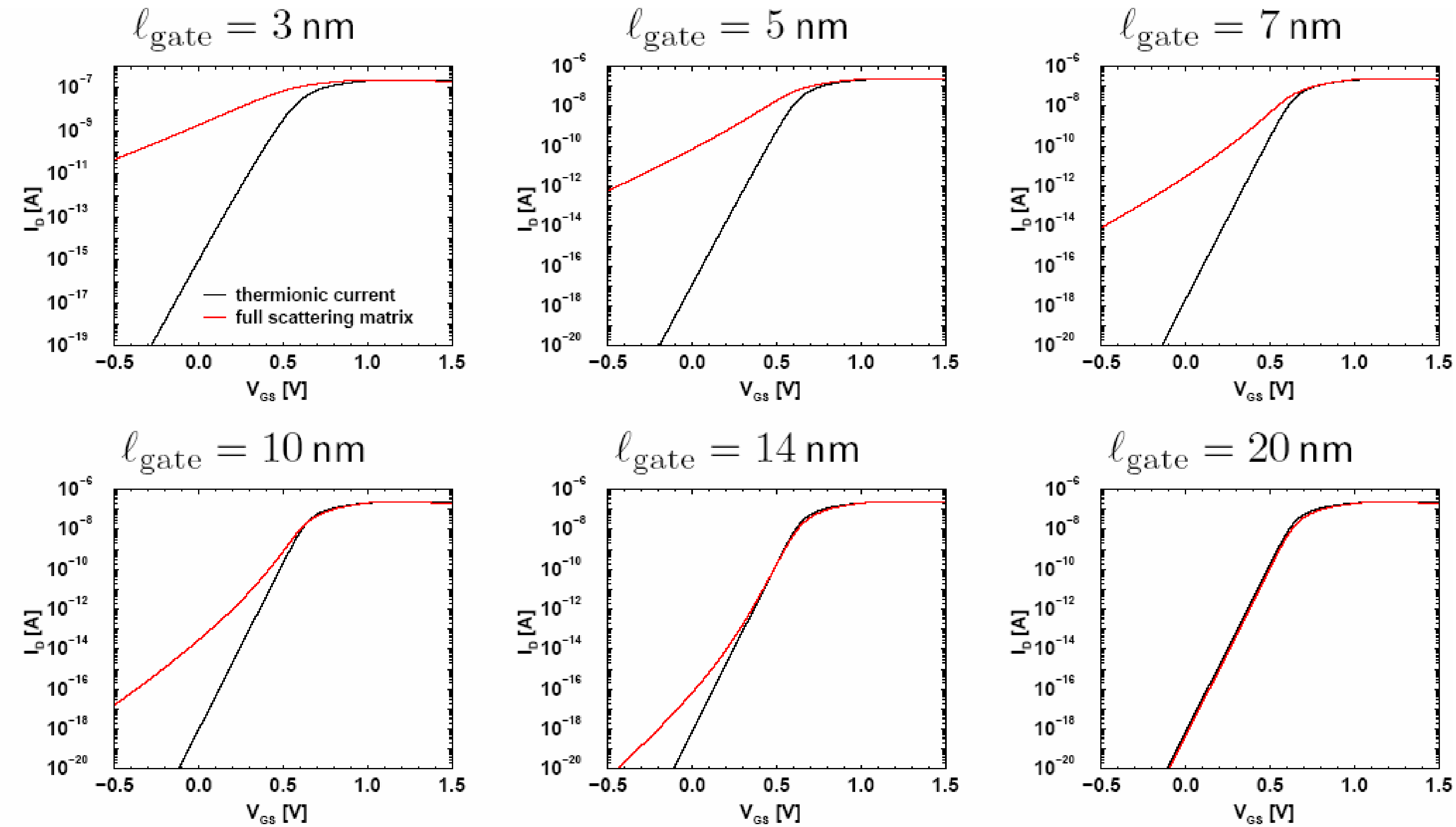
$$I = -\frac{2e}{h} \sum_{v,i} \int_{\epsilon^0_{v,i}}^{\infty} \mathrm{d}\epsilon \, T_{v,i}(\epsilon) \Big(f\big(\beta(\epsilon - \epsilon^{\mathrm{src}}_{\mathrm{Fermi}})\big) - f\big(\beta(\epsilon - \epsilon^{\mathrm{drn}}_{\mathrm{Fermi}})\big) \Big) \qquad \text{1D}$$

$$I = -\frac{2e}{h} \sqrt{\pi} \frac{W}{\lambda_{\mathrm{th}}} \sum_{v,i} \int_{\epsilon^0_{v,i}}^{\infty} \mathrm{d}\epsilon \, T_{v,i}(\epsilon) \Big(\mathfrak{F}_{-\frac{1}{2}}\big(\beta(\epsilon^{\mathrm{src}}_{\mathrm{Fermi}} - \epsilon)\big) - \mathfrak{F}_{-\frac{1}{2}}\big(\beta(\epsilon^{\mathrm{drn}}_{\mathrm{Fermi}} - \epsilon)\big) \Big) \qquad \text{2D}$$

W: width of the device

λ_{th}: electron thermal wave–length $h/\sqrt{2m^* k_{\mathrm{B}} T}$

Source–Drain Tunneling in nano–MOSFETS



double–gate MOSFETs with a Si body thickness of 1 nm ($V_{sd} = 1\,\mu$V).

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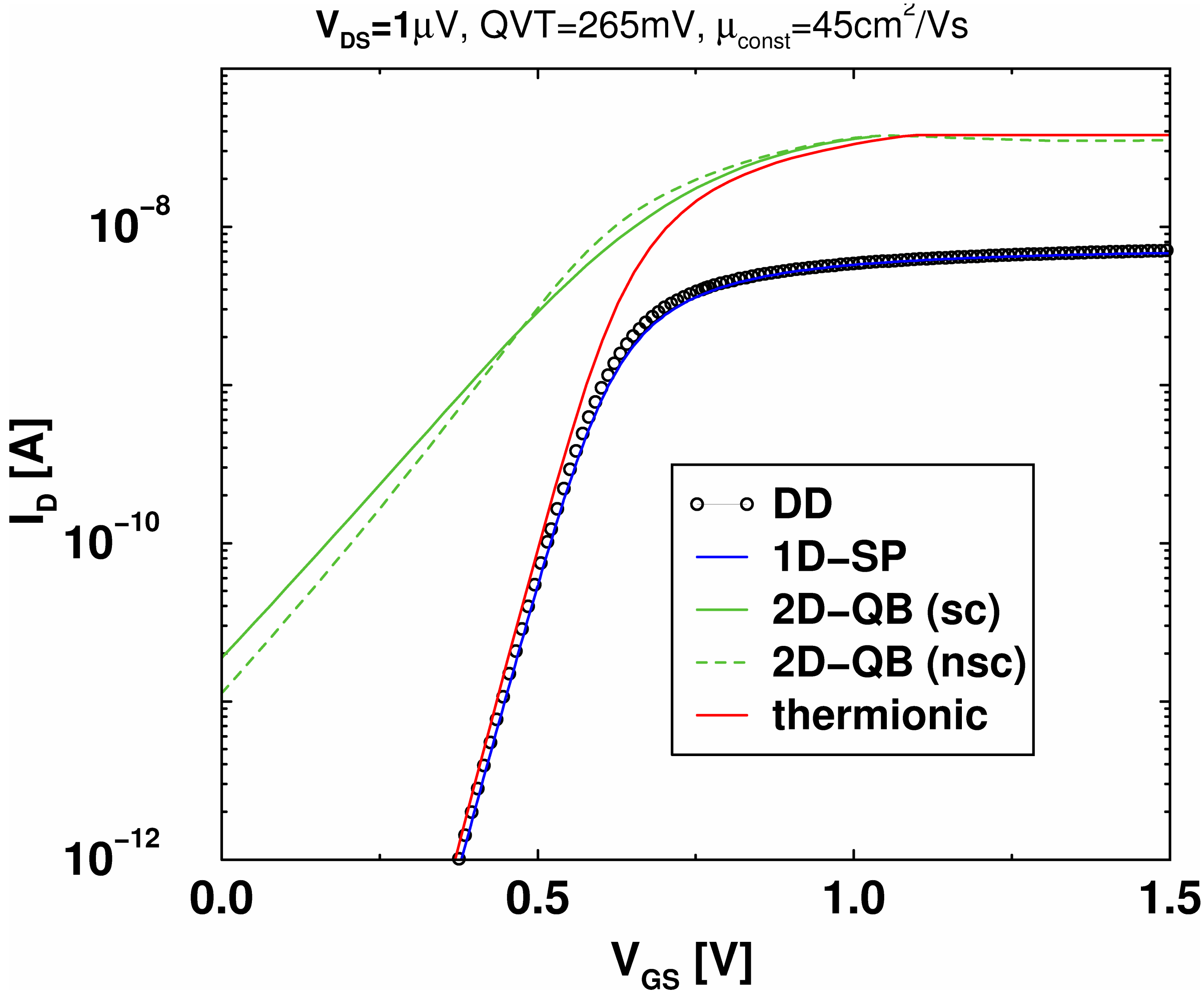
Model comparison (L_{gate} = 5nm)



Simulation of Quantum–Dot Flash RAM

⇝ Challenge: Devices with quantum dots **and** classical channels.

× **SIMNAD** cannot handle dissipative transport . . .

✓ . . . but **DESSIS** can !

DESSIS has a 1D Schrödinger solver and a QDD facility, but

× it cannot handle multi–dimensional confinement properly. . .

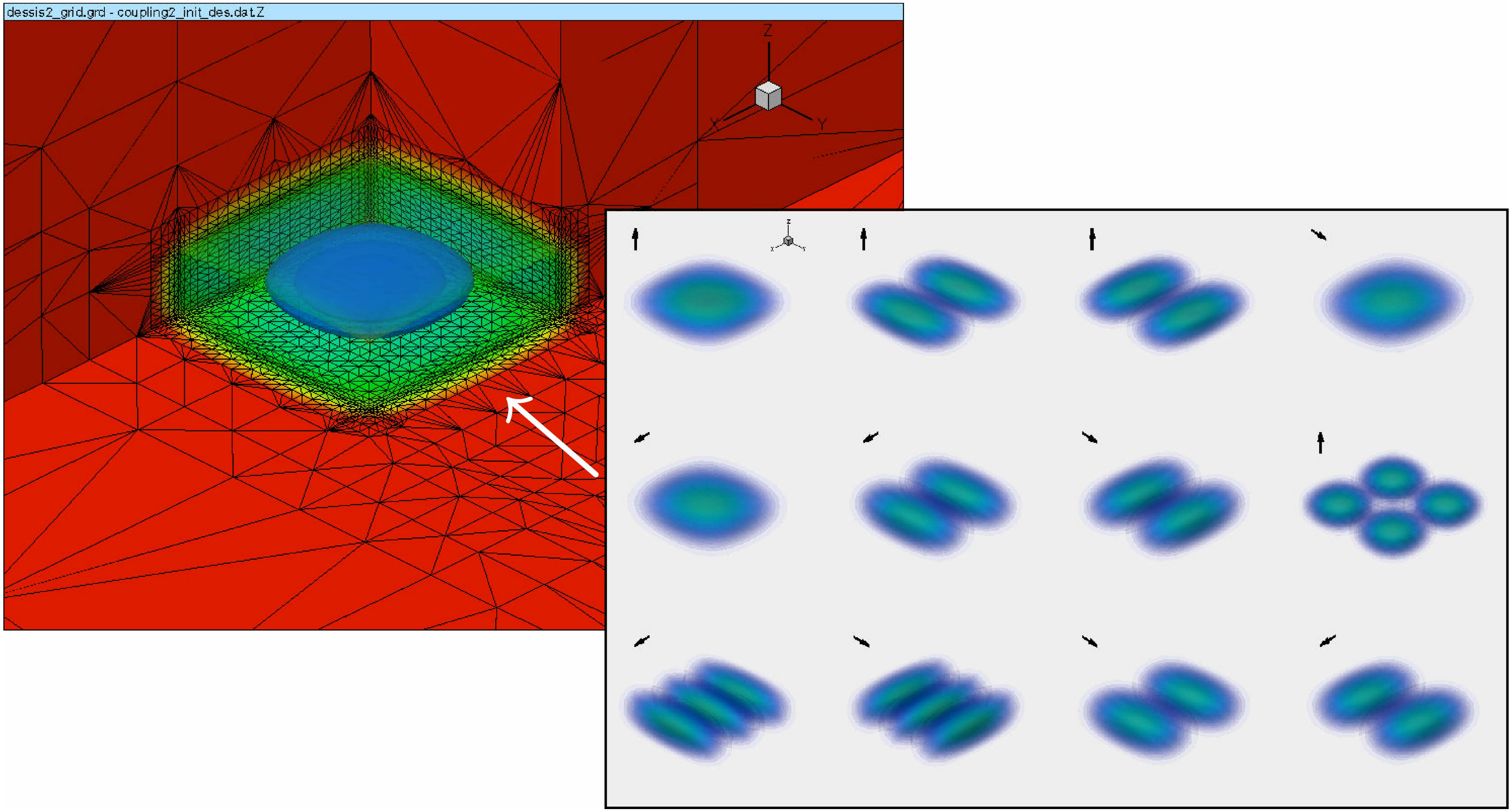
✓ . . . but **SIMNAD** can !

⋆ **Together, the two simulators can do both !**

⇒ Apply a simulator coupling scheme !

Coupled DESSIS/SIMNAD Simulations

Simulator coupling: **SIMNAD** charge density on **DESSIS** mesh:



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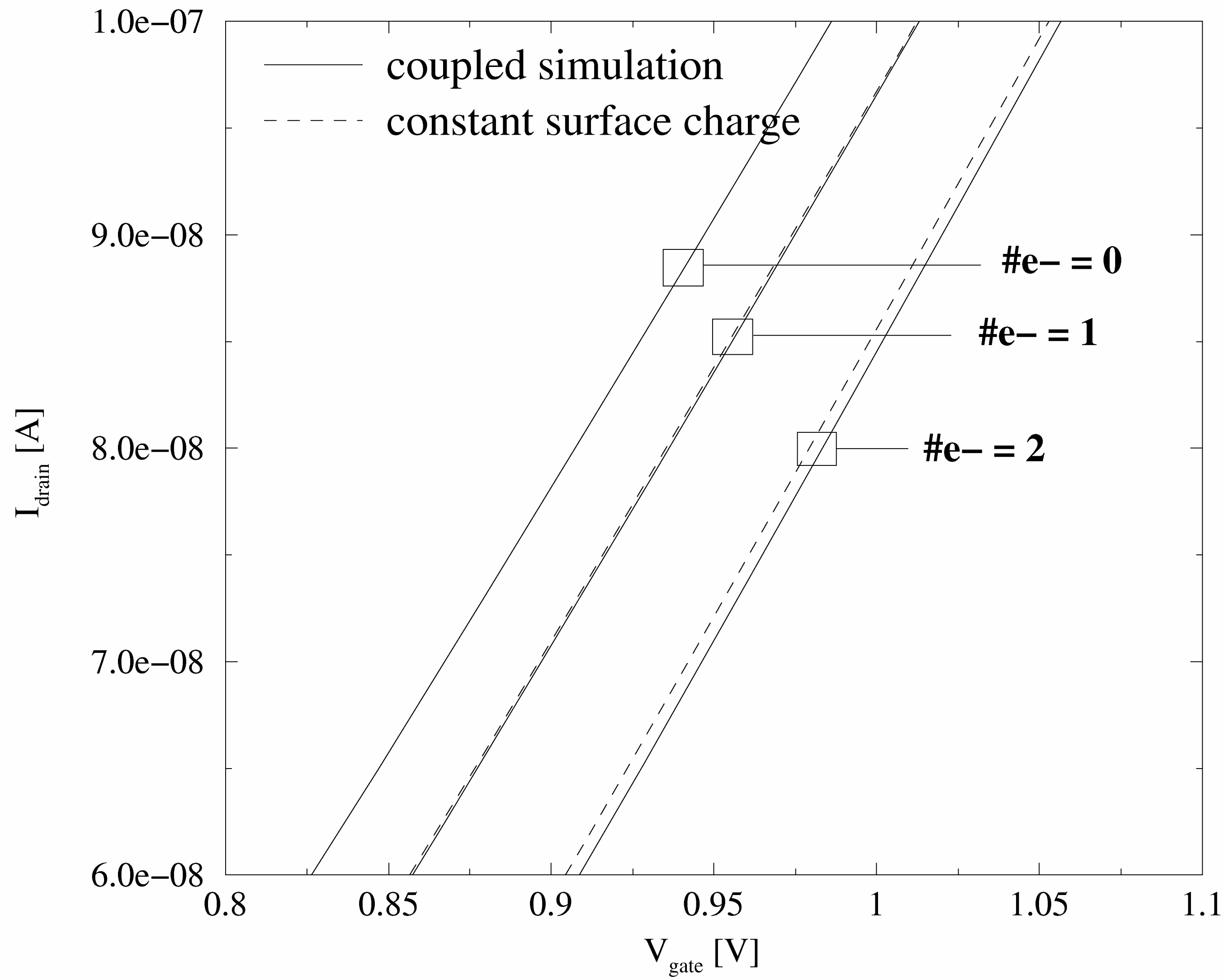
Coupled DESSIS/SIMNAD Results



Conclusion

- ★ Downscaling of devices ⇒ non–local phenomena
- ★ Two kinds of non-localities
  - classical: ballistic transport; non-local μ
  - quantum: wave-nature of the carriers
- ★ classical non-localities: full band MC ☺
- ★ quantum mechanics: ☺/😐
  simplifications necessary (high comp. effort)
- ★ DESSIS/SIMNAD coupling:
  quantum dots **and** classical channels in one device

Acknowledgments

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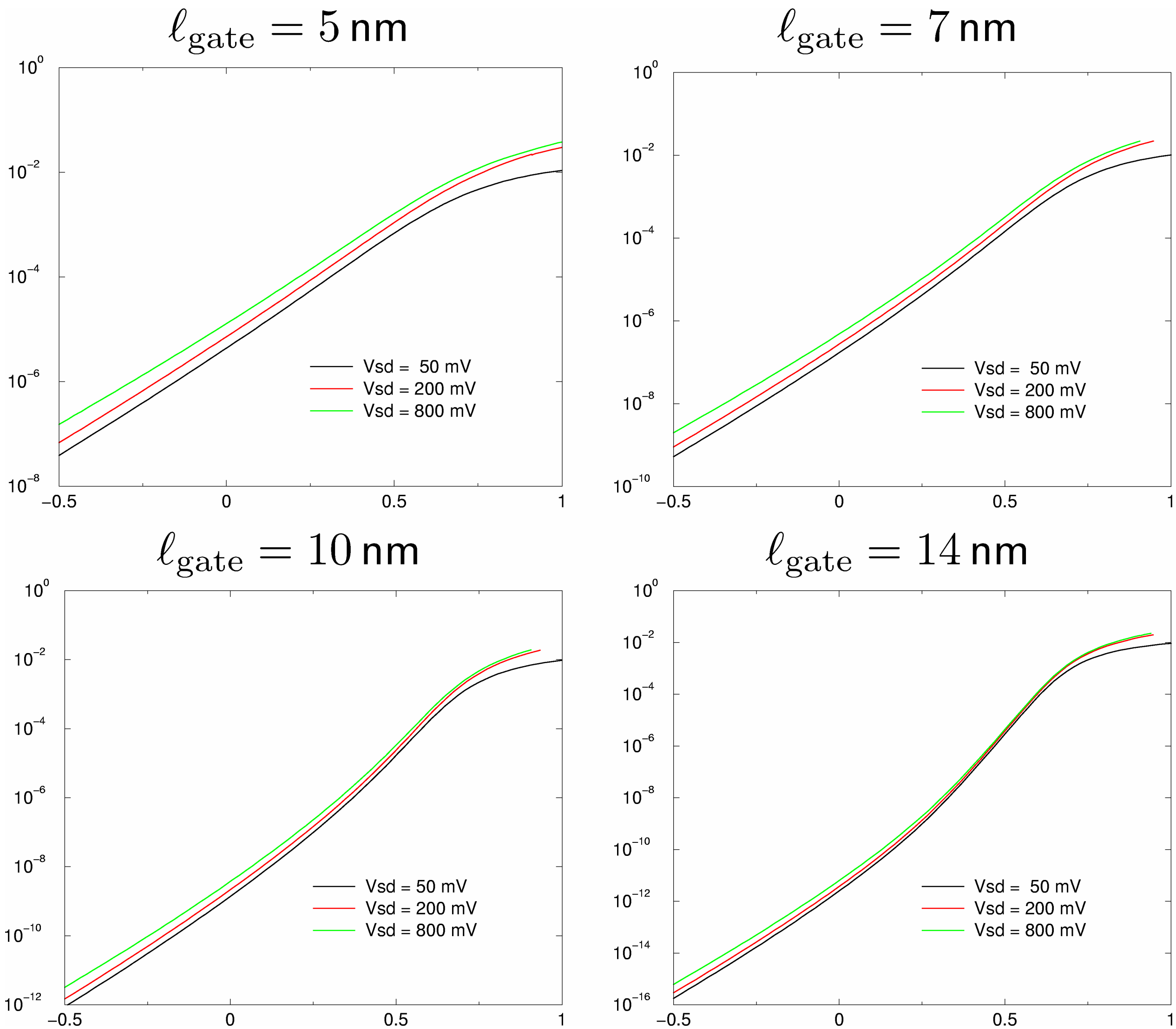
The work on Monte–Carlo simulation was partially funded by the Swiss "Kommission für Technologie und Innovation" (KTI).

Thank you !

Ballistic MOSFET under forward bias



Quantum ballistic current for different source–drain voltages [in A/μm]