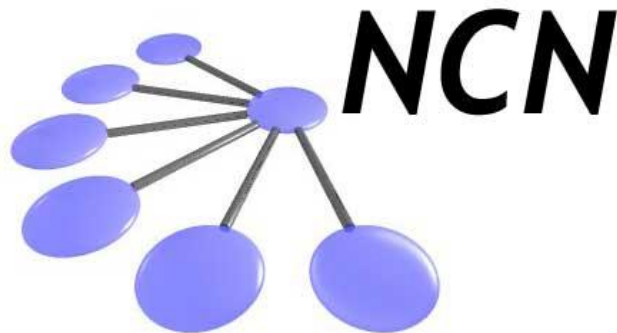


Network for Computational Nanotechnology (NCN)

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OMEN Nanoiwire* Supporting Document Limitation of the Tool at Large Gate Voltage



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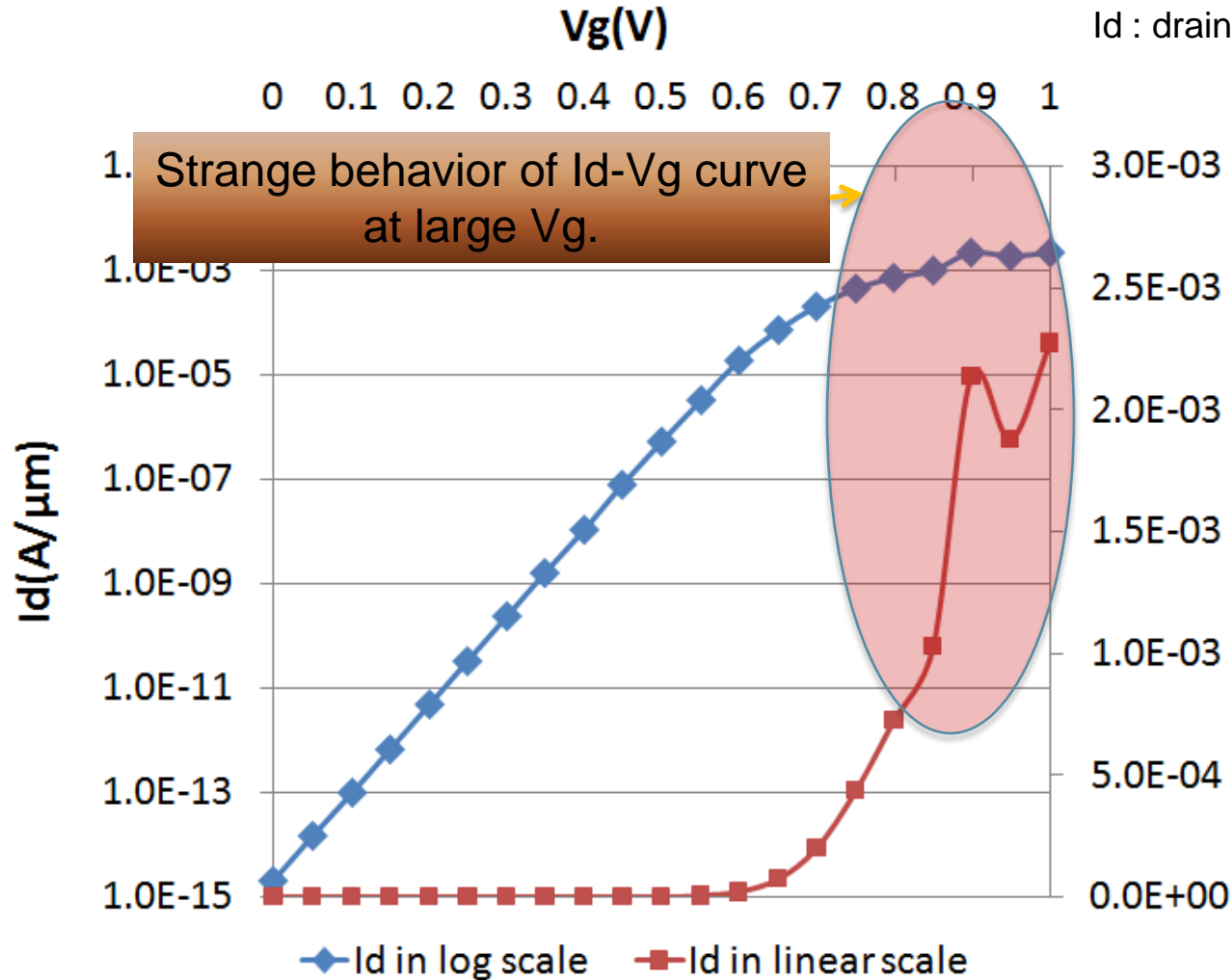
What if a user wants to simulate a nanowire FET at large gate bias to obtain its on-current* using OMEN Nanowire?

Then, the I_d - V_g curve at high gate voltage is required.

*On-current is defined as the drain current at $V_g = V_{dd}$ where V_{dd} is positive supply voltage (<http://en.wikipedia.org/wiki/Vcc>). On-current is the measure of how fast the device can operate.

Problem in Id-Vg Characteristics

Id : drain current , Vg : gate voltage



Circular
Silicon Nanowire

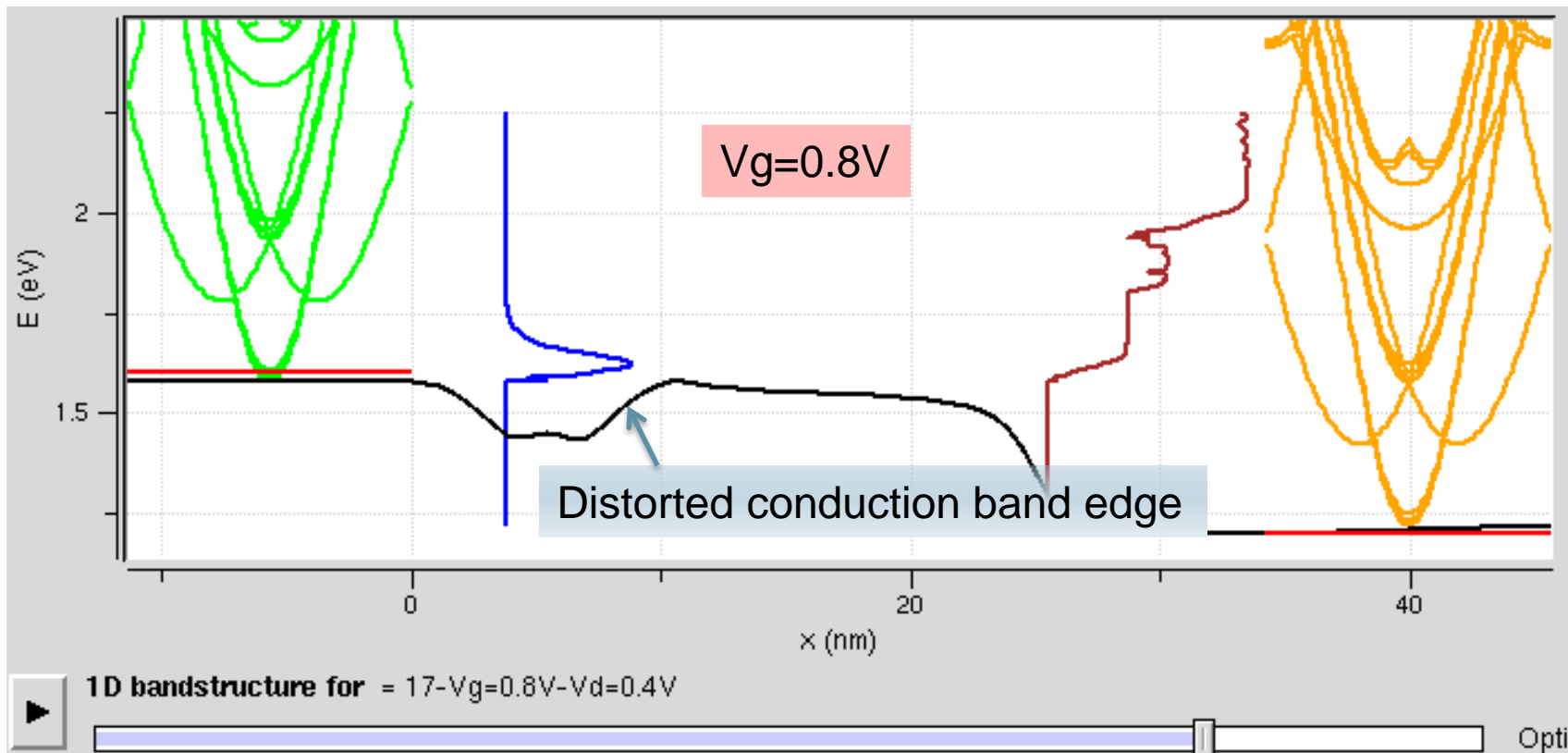
Dch* : 2nm
Lch** : 15 nm
 χ_{ch}^\dagger : 4.05eV
 ϕ_{ch}^\ddagger : 4.25eV

*Dch : diameter of nanowire **Lch : channel length

$\dagger\chi_{ch}$: affinity of the channel material $\ddagger\phi_{ch}$: gate work function

Bandstructure*

*Explanations of the plot below can be found in the first time user guide of OMEN Nanowire



- According to the bandstructure plot, problems occur at $V_g=0.8V$.
- Users need to look into the output log and input deck for a more detailed description of the simulation process

1. Find the following script in the inputdeck

Inputdeck is a part of output plots

```

Result: Output Log
poisson_iteration = 15; //number of poission iteration
poisson_criterion = 1e-3; //criterion for convergence of poission iteration
Assemble Hamiltonian
Solve Linear System
Extract Data=5.055151e-01 [s]
Solving Poisson Equation
Poisson Inner Loop 1: 4.613874e-02
Poisson Inner Loop 2: 2.826435e-02
Poisson Inner Loop 3: 1.750554e-04
Solving Poisson Equation took 5.170729e-01 [s]
Vg: 8.000000e-01, Vs: 0.000000e+00, Vd: 4.000000e-01 Iteration 15: 2.905393e-02, Duration: 4.090117e+01 [s]
Point: 0 / Group: 0
Boundary Conditions=9.513979e-01 [s]
Assemble Hamiltonian=0.000000e+00 [s]
Vg = 0.8V, Vs = 0V, Vd=0.4V
Boundary Conditions=9.732540e-01 [s]
Assemble Hamiltonian=2.226379e-01 [s]
Solve Linear System=3.596459e+00 [s]
Extract Data=8.861709e-02 [s]
Point: 128 / Group: 0
Boundary Conditions=9.167311e-01 [s]
Assemble Hamiltonian=2.309129e-01 [s]
Solve Linear System=3.637773e+00 [s]

```

2. Look into "Output log". You can scroll up and down to find where the problem happens

Residue

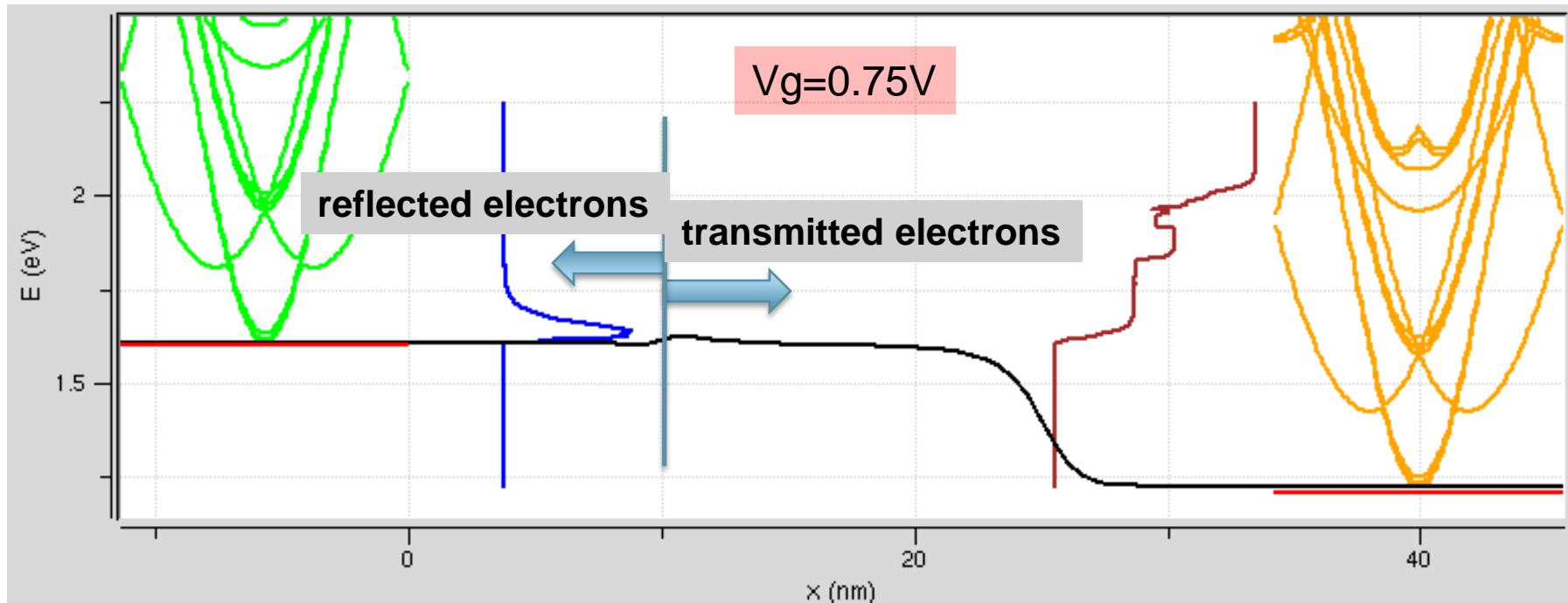
3. Residue is larger than the criterion in the inputdeck whereby the iteration reached its maximum, 15.

→ **Problem!!**
Poisson equation isn't converged*

n.b.) Poisson and Schrödinger equations are solved self-consistently to obtain the electron density and electrostatic potential in the nanowire.

***"Converge" means that the residue of the solution of Poisson equation become smaller than the convergence criterion

Physical Meaning

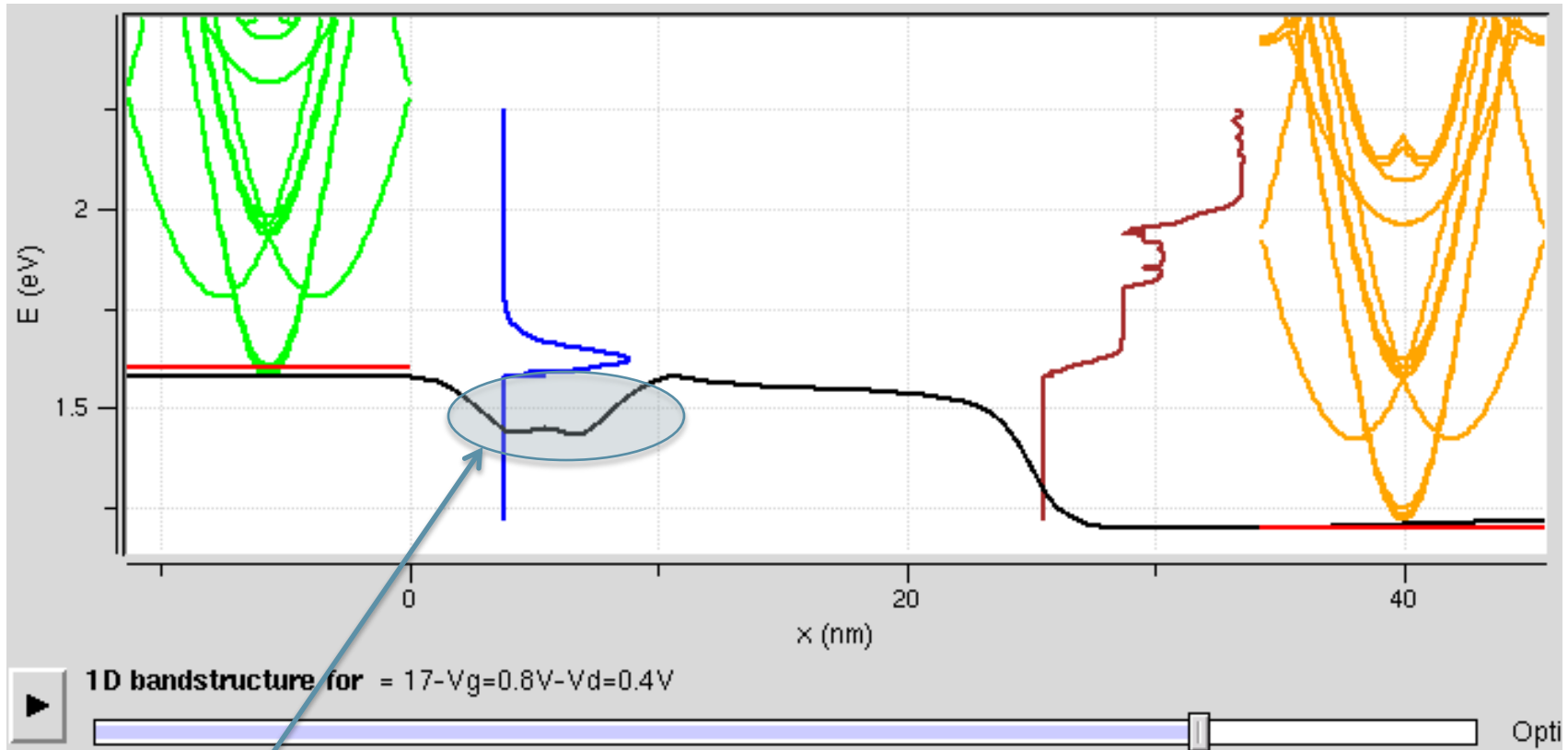


- At high gate voltage, the barrier height* in the channel becomes very small
- The number of electrons reflected back at the barrier are too small.
- The equilibrium in the source region** cannot be achieved.
- Poisson equation cannot converge.

*The barrier height is related to the workfunction of the gate and the affinity of the channel material

**Equilibrium in the source : the number of electrons = the number of donors

Forcing Equilibrium



- So potential distortion occurs to achieve equilibrium at the source end.
- Raising the convergence criterion in such a situation does not help.
- The calculated drain current is not correct and has no meaning.
- This effect is inherent to ballistic transport and is not specific to OMEN.

- The reason for the strange behavior of I_d - V_g curve at high gate voltage is investigated
- The high gate voltage causes barrier height to be lowered to some degree that the equilibrium in the source region cannot be achieved easily.
- Poisson solver in OMEN attempts to distort(lower) the conduction band edge of the source end to achieve equilibrium.
→ Drain current is changed or distorted due to this behavior.
- The plotted drain current is not correct when Poisson equation does not converge.
- Users need to be careful about the results at high gate voltages.
→ Input deck and output log files should be carefully investigated