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Silicon to Software™

New framework in QuantumATK for smart and efficient simulation of device characteristics.

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Outline

- Atomistic device simulations using QuantumATK.
- The *study object* concept.
- The IV Characteristics study object.
- Creating a FET device using QuantumATK: silicon-on-insulator (SOI).
- Running the IVCharacteristics simulation.
- Analyzing the SOI device using the IV Characteristics analysis tool.
- Conclusions.

Industrial publications with QuantumATK

First-principles investigations of TiGe/Ge interface and recipes to reduce the contact resistance

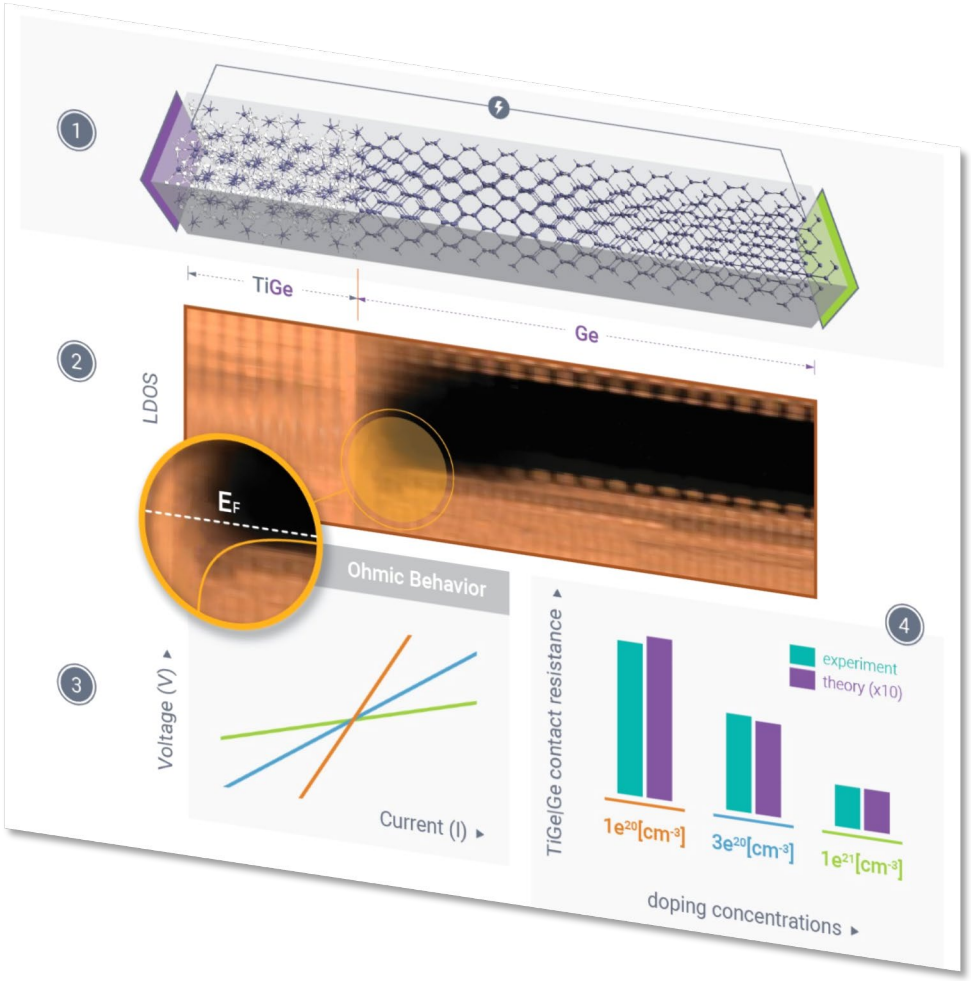
Study by GlobalFoundries & IBM Research

Dixit et al., IEEE Trans. Elec. Dev. **64**, 3775 (2017)

Probing the intrinsic limitations of the contact resistance of metal/semiconductor interfaces through atomistic simulations

Study by Imec, University of Antwerp, KULeuven, MathAM-OIL and Synopsys QuantumATK Team

Pourtois et al., ESC Trans. **80**, 303 (2017)



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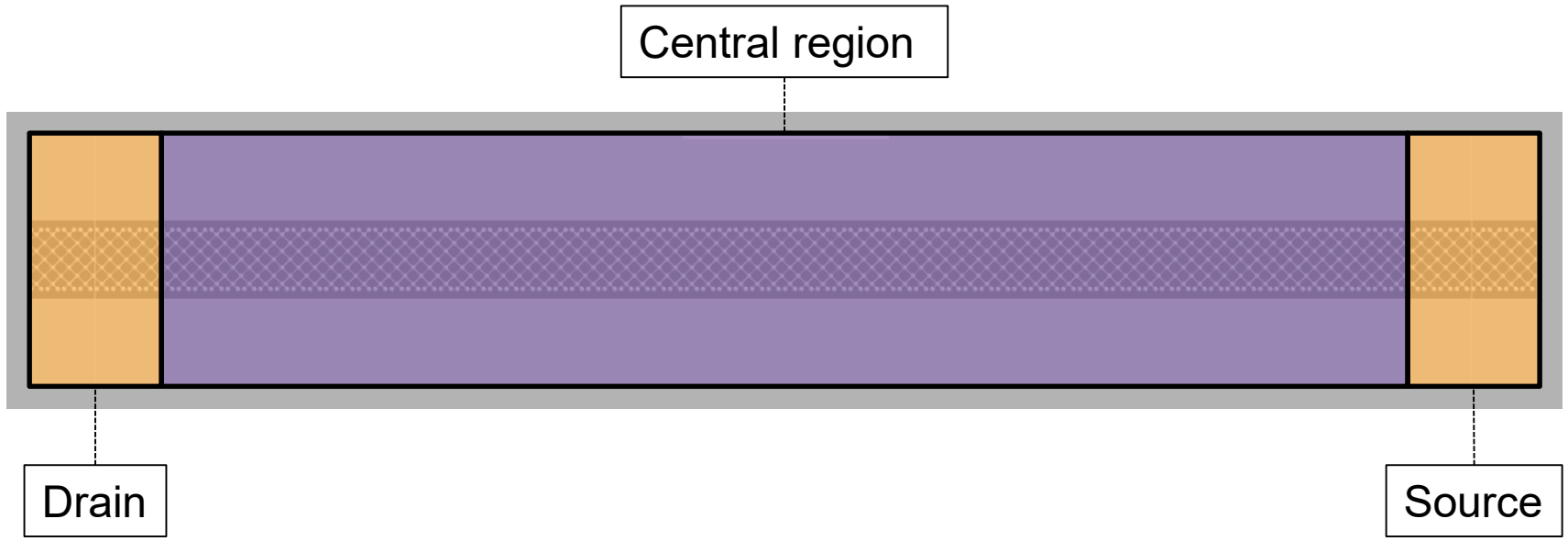
Simulating atomistic devices using QuantumATK.



- The NEGF framework implemented in QuantumATK allows one to calculate the electronic properties of a central region connect to semi-infinite source and drain electrodes.

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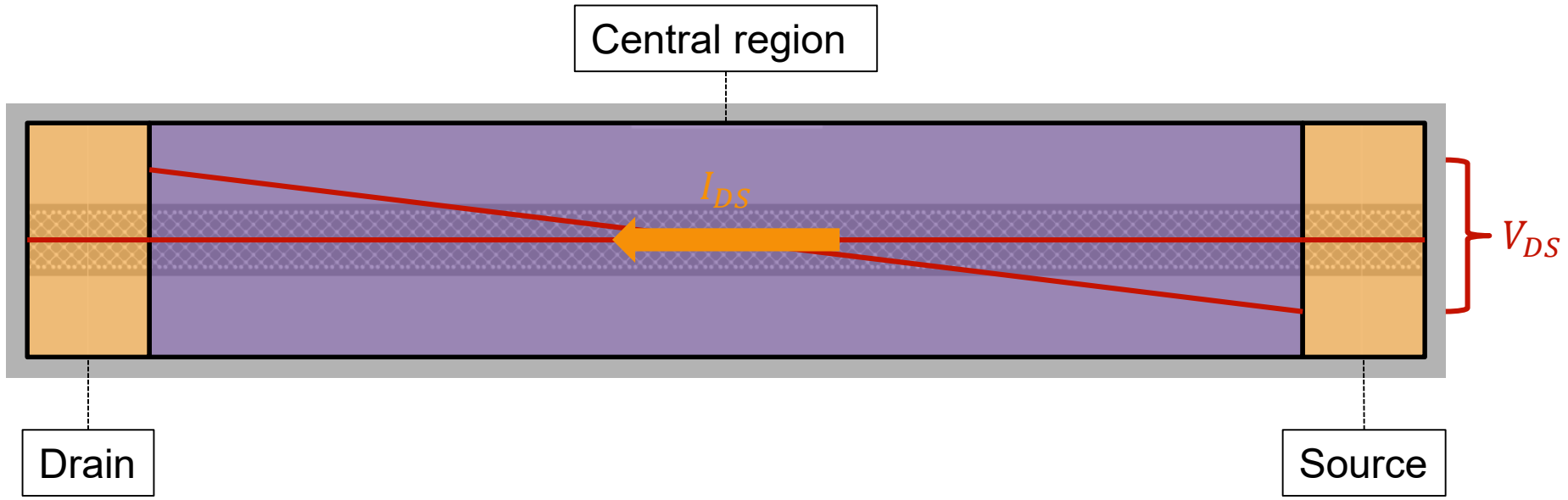
Simulating atomistic devices using QuantumATK.



- The NEGF framework implemented in QuantumATK allows one to calculate the electronic properties of a central region connect to semi-infinite source and drain electrodes.
- A voltage bias can be applied between the electrodes in order to calculate the drain-source current.

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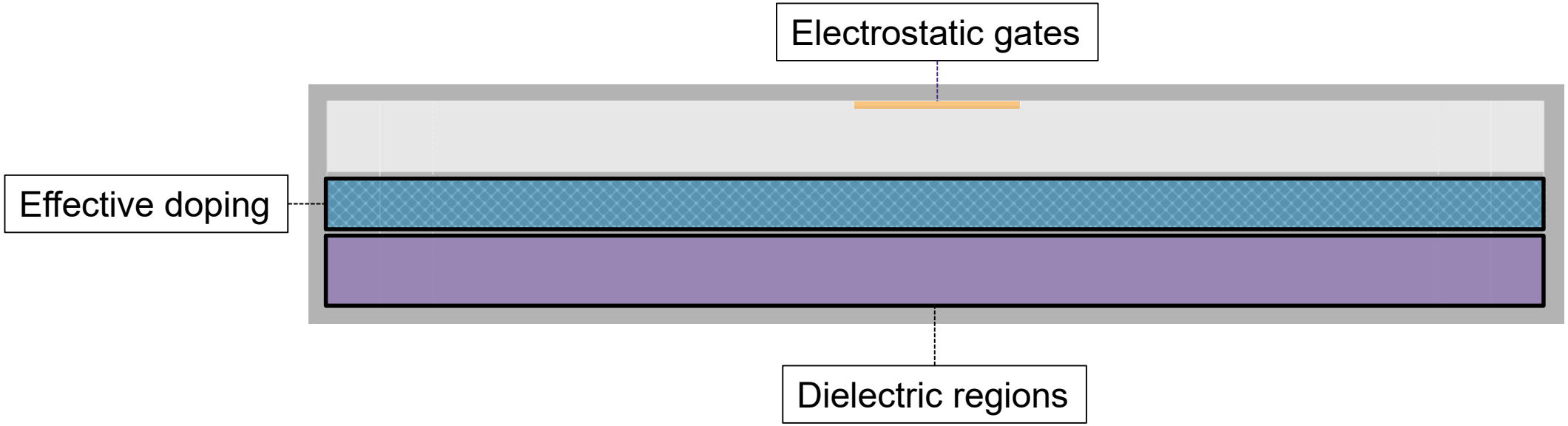
Simulating atomistic devices using QuantumATK.



- An effective doping scheme can be used to simulate doped semiconductors.
- Electrostatic metallic gates can be added to modulate the channel region.
- Dielectric region can be used to simulate encapsulating oxides.

This framework allows one to simulate IV characteristics of devices.

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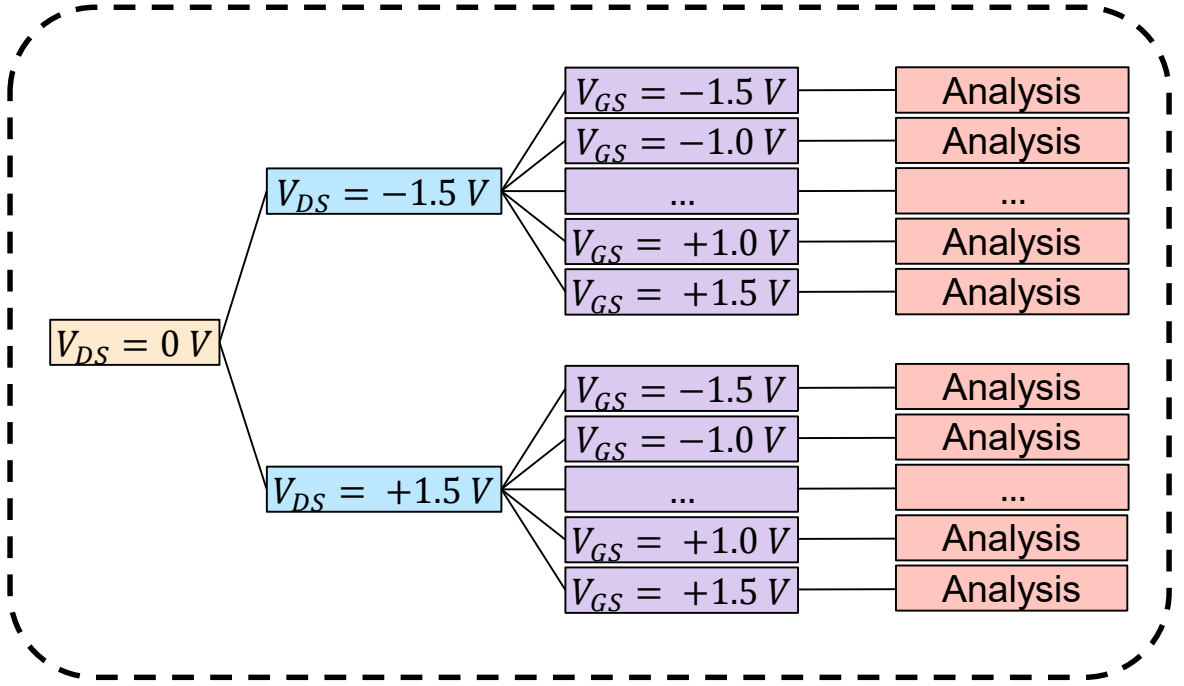
Study objects make life easier for …

…complex simulation workflows made of many smaller and independent tasks .

Device electrical characteristics



IV Characteristics study object

More info at: *docs.quantumwise.com/manual/includes/Study.html*

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The IV Characteristics study object…

…can be used to perform a detailed study on the electrical characteristics of atomic-scale devices, by performing automatic scans over:

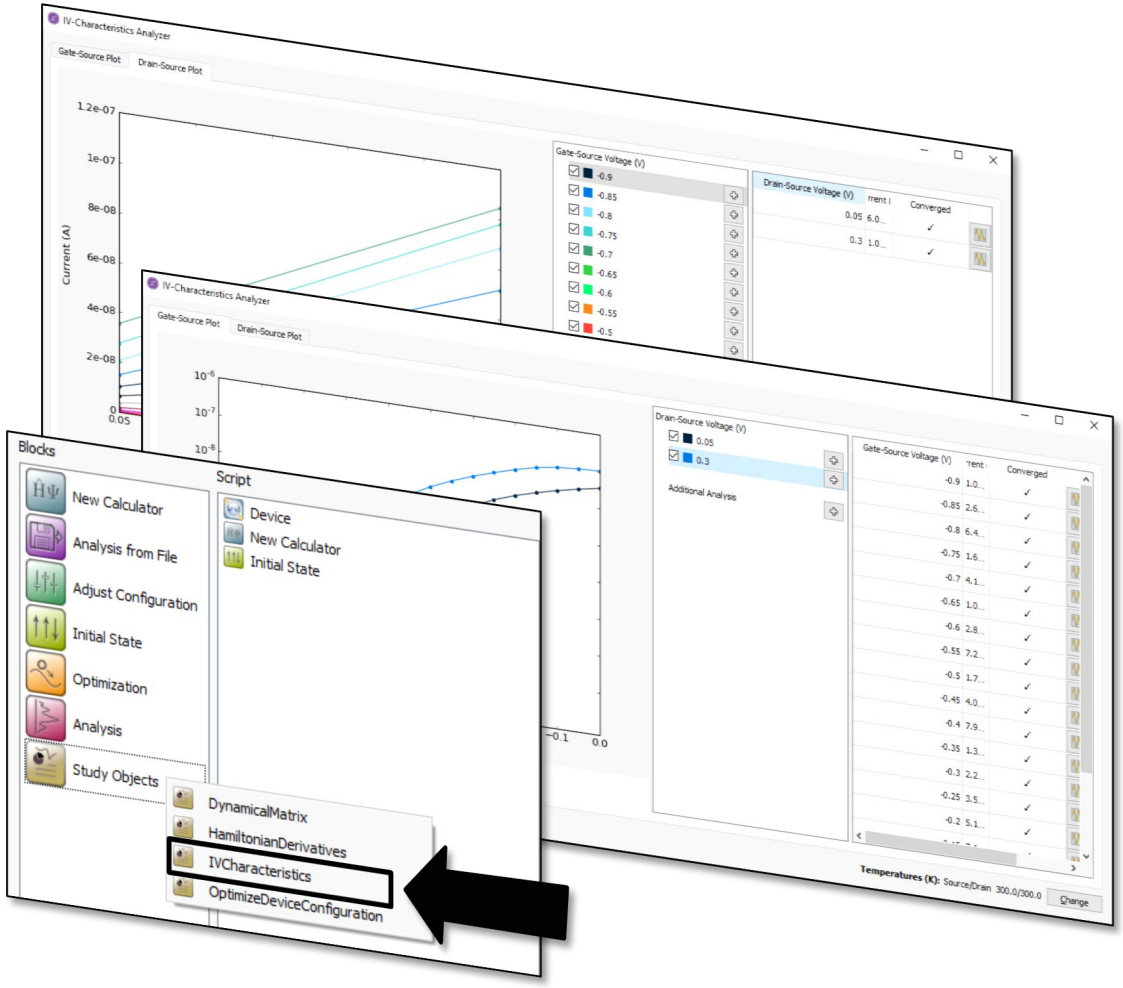
- The *Drain-Source (DS) voltages*.
- The *Gate-Source (GS) voltages*.

…uses a smart restart strategy to figure out the best starting guess and facilitate convergence of device calculations at finite DS and GS voltages.

…allows the user to extend the range of the simulation by adding additional data points in a seamless manner.

…allows one to calculate several electrical characteristics of the device:

- *On/Off ratio*.
- *Sub-threshold slope*.
- *Drain-Source saturation voltage*.
- *Drain-induced barrier lowering*.
- *Transconductance*.



More info at: *docs.quantumwise.com/manual/Types/IVCharacteristics/IVCharacteristics.html*

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Creating a FET device using QuantumATK: silicon-on-insulator (SOI).

1 - Creating the silicon slab.

2 - Creating the FET channel region.

3 - Creating the FET device configuration.

3.1 - The doping profile affects the device characteristics.

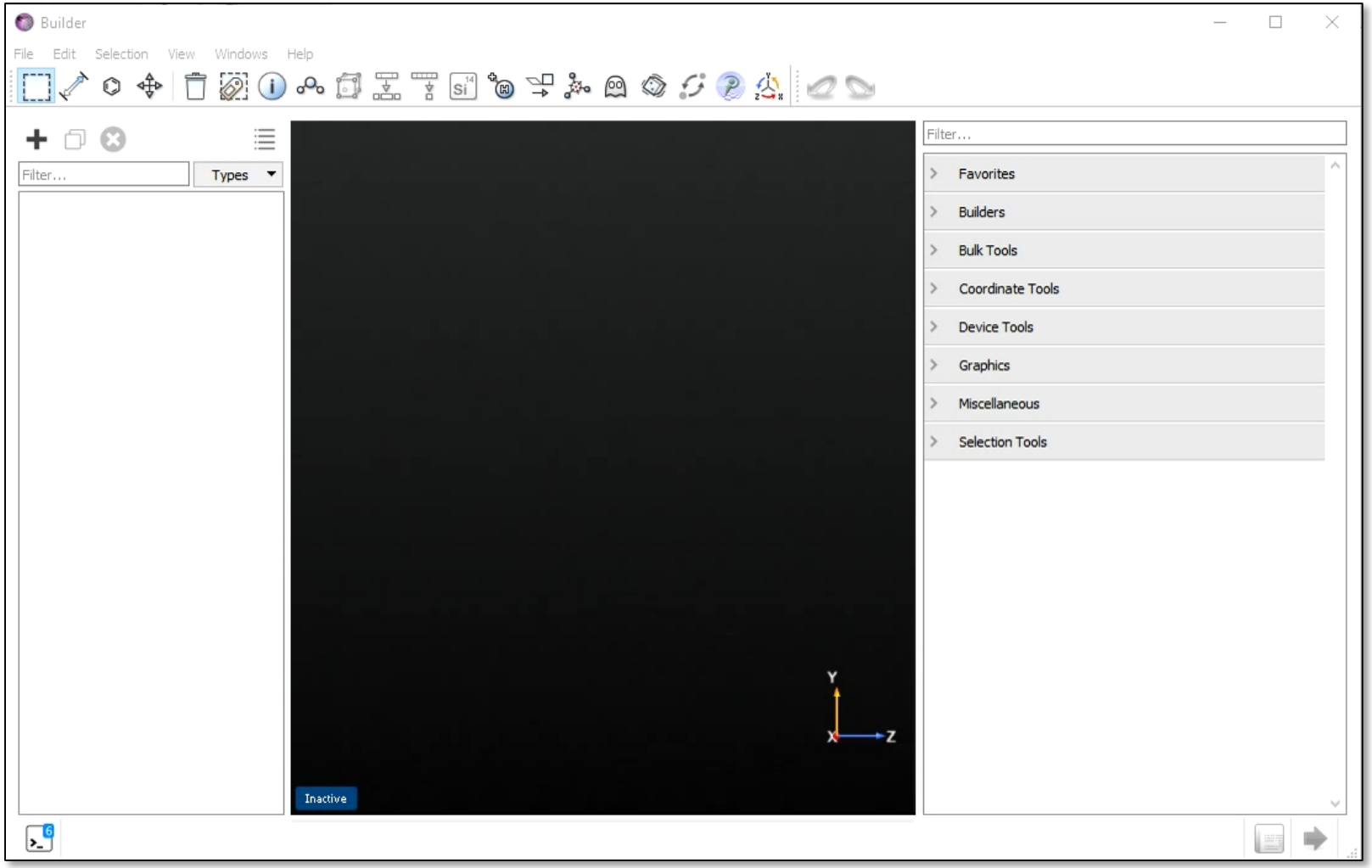
1 - Creating the silicon slab.

A silicon slab is created in the **NanoLab Builder** by:

1. Retrieving the Silicon unit cell from the **Database**.

2. Using the **Builder plugins** to modify the structure:
   - *Supercell*
   - *Surface (cleave)*
   - *Lattice parameters*
   - *Center*
   - *Passivation tool*
   - *Swap axes*

The plane of the silicon slab has to be oriented along the C direction of the unit cell.



More info at: *docs.quantumwise.com/tutorials/ivcharacteristics/ivcharacteristics.html*

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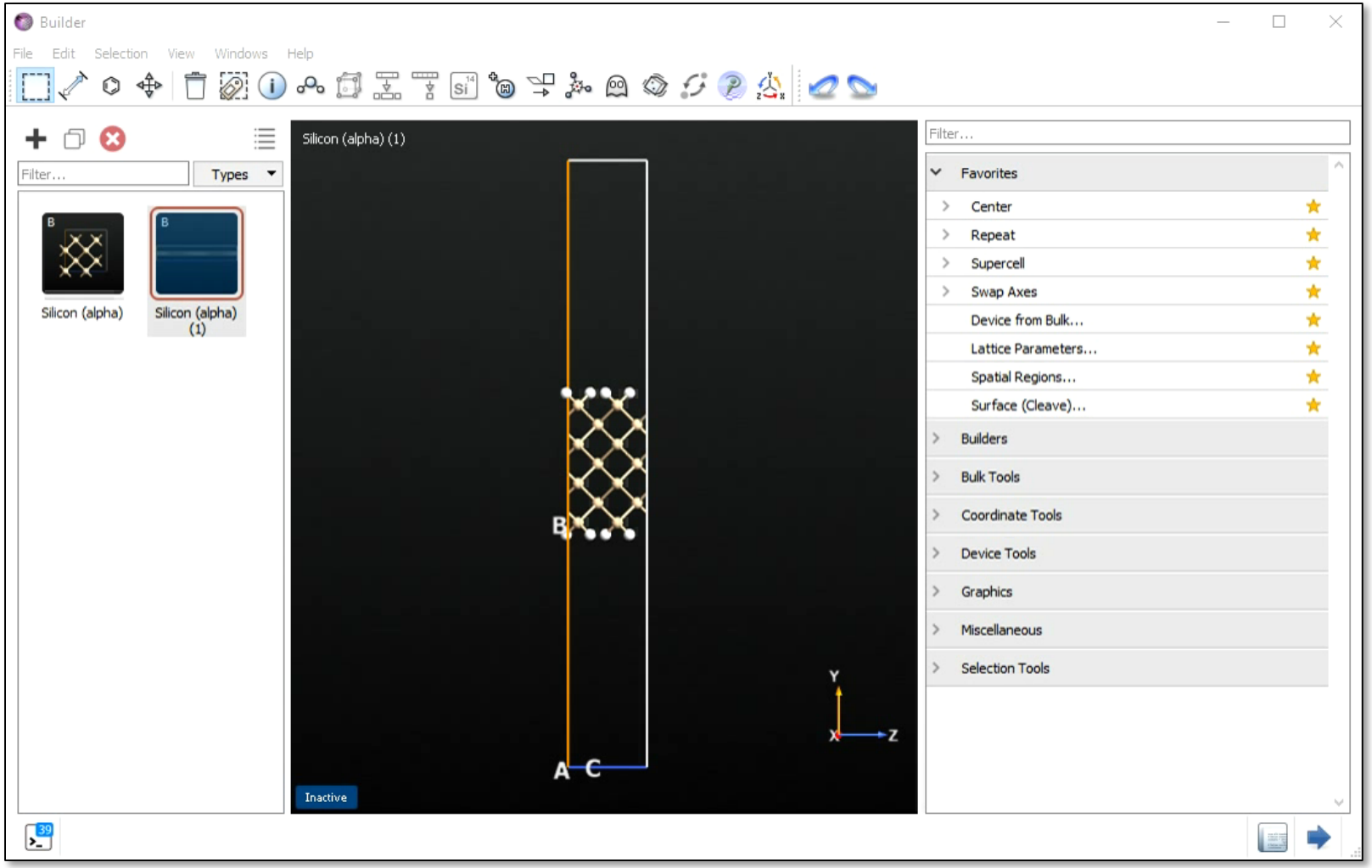
2 - Creating the channel region.

The **bulk configuration** of the FET channel is created by:

1. Repeating the structure in the C direction using the *Repeat* plugin.

2. Adding the gate and dielectric above and below the silicon slab by using the *Spatial regions* plugin.



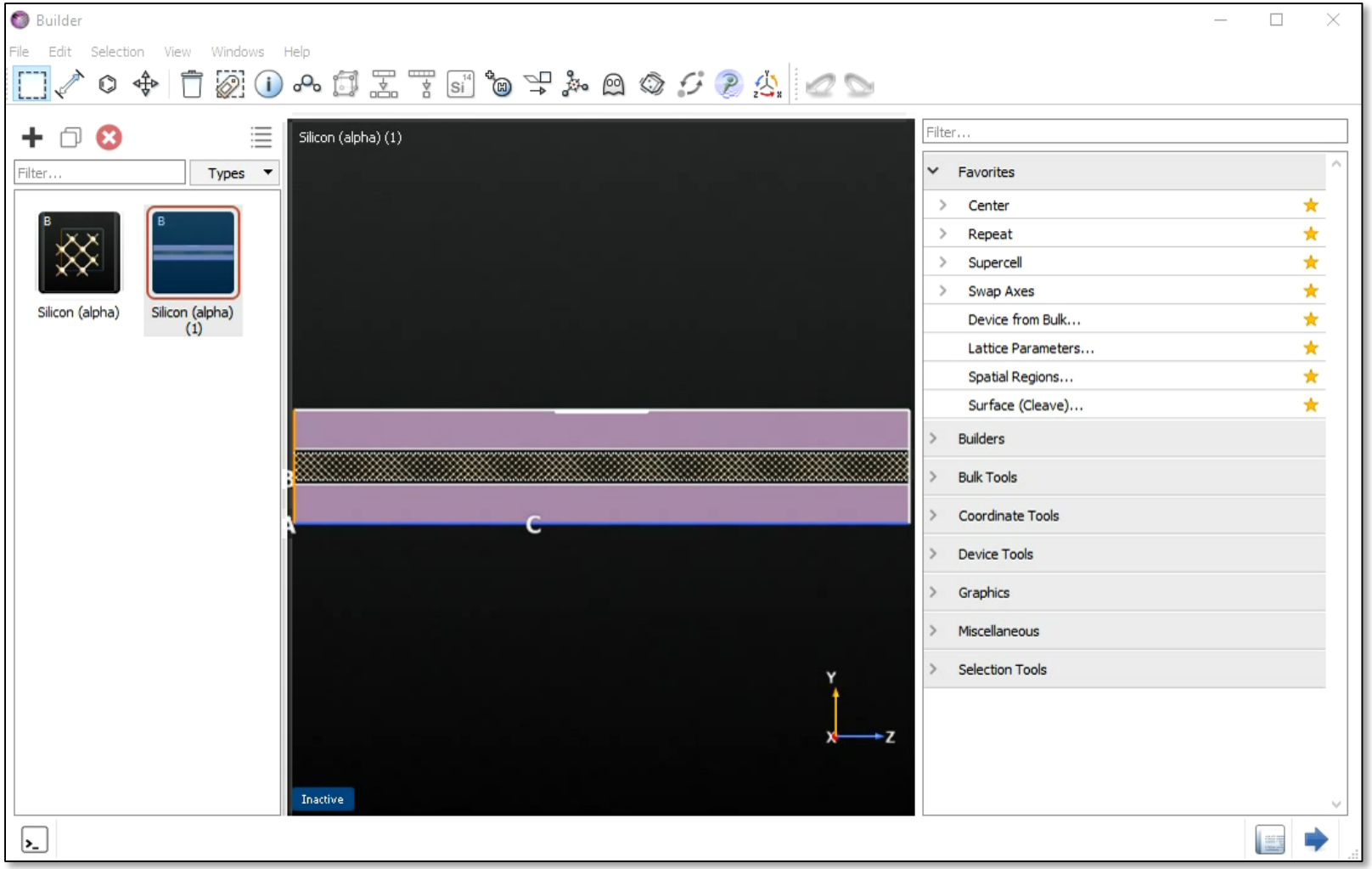
More info at: *docs.quantumwise.com/tutorials/ivcharacteristics/ivcharacteristics.html*

3 - Creating the device from the channel region.

The FET **device configuration** is created from the bulk configuration by using the *Device from Bulk…* plugin.

The *Device from Bulk…* plugin allows one to choose the length of the electrode repetition.

The **minimal electrode concept** alleviates this problem by automatically repeating the electrode electronic structure.



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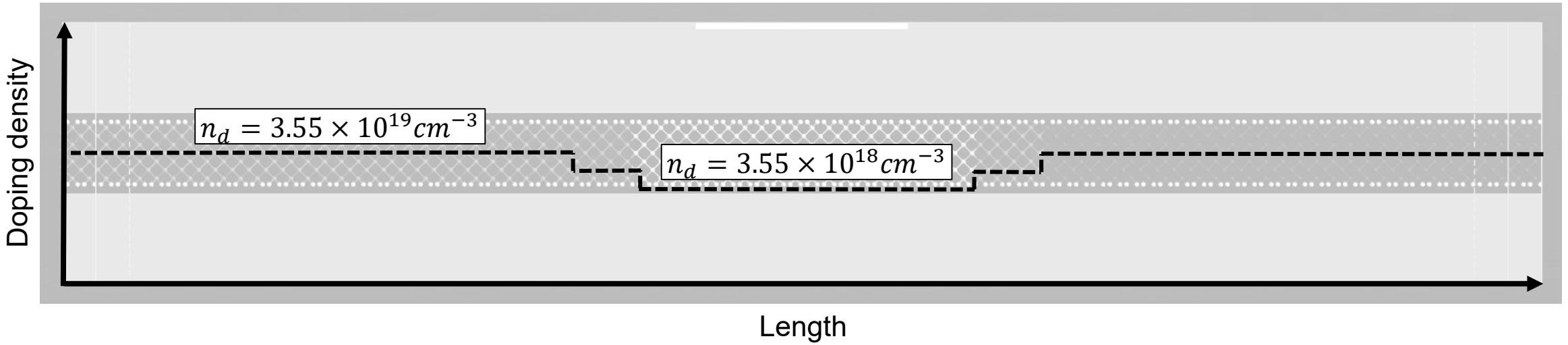
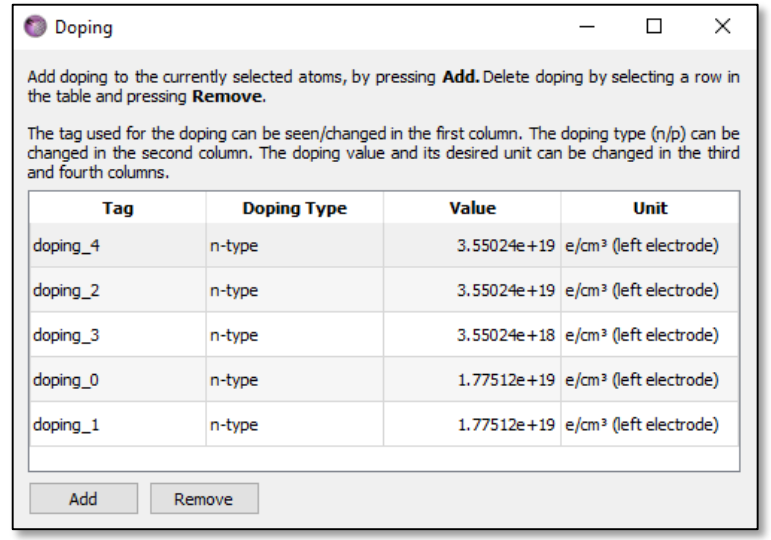
3.1 - The doping profile affects the device characteristics



The **doping profile** can be set using the *Doping* plugin in the Builder.

Electrical parameters such as the subthreshold swing and the drain-induced barrier lowering are extremely sensitive to the doping profile.



More info at: *docs.quantumwise.com/tutorials/ivcharacteristics/ivcharacteristics.html*

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Running the IV Characteristics simulation.

1 - Setting up the QuantumATK script.

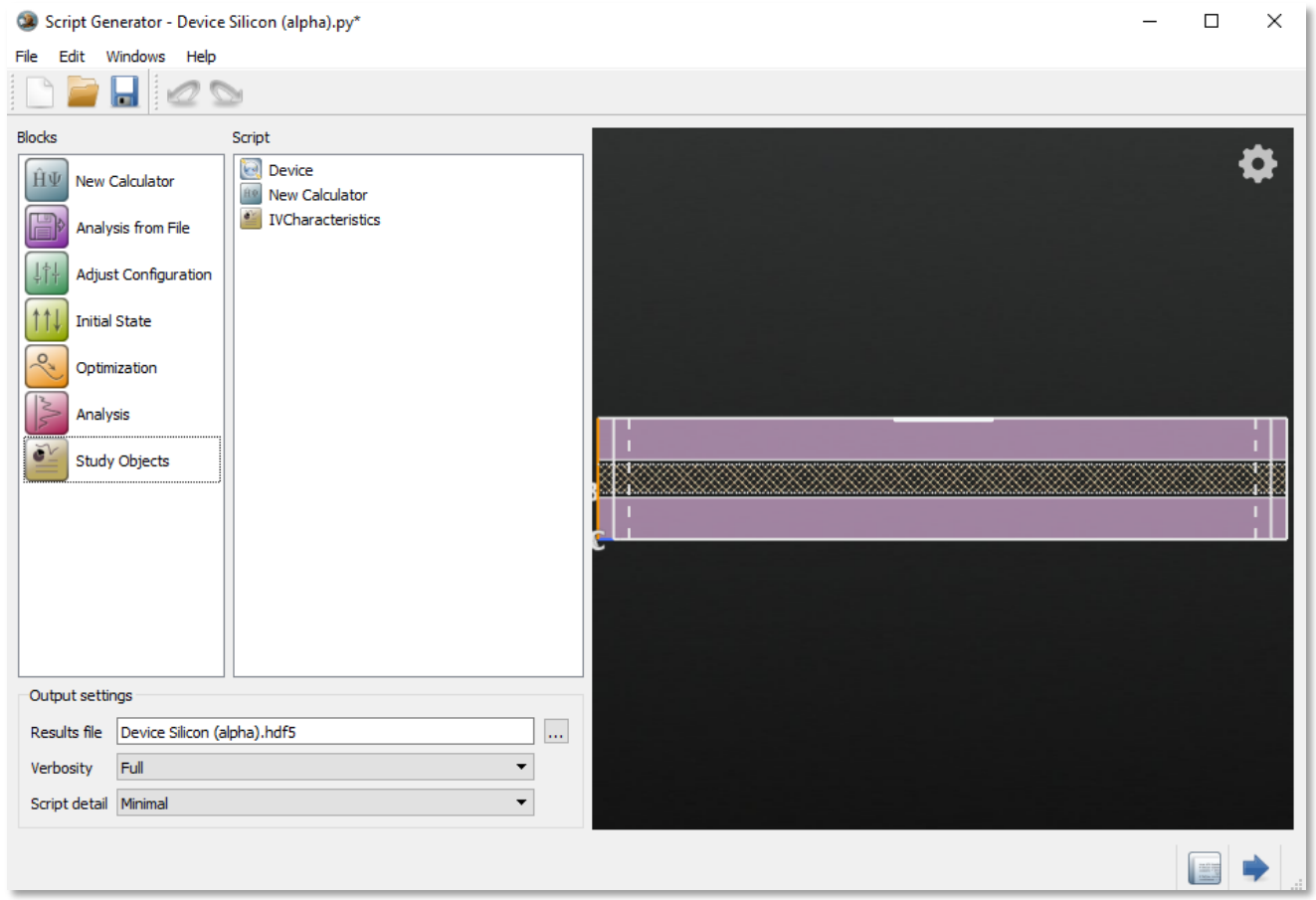
1.1 - A closer look at the IV Characteristics window…

2 - Inspecting the log file.

1 - Setting up the QuantumATK script.

The device configuration is send to the **Script Generator**, where the calculation script is created by adding:

- A new calculator block
- An **IVCharacteristics** block



More info at: *docs.quantumwise.com/tutorials/ivcharacteristics/ivcharacteristics.html*

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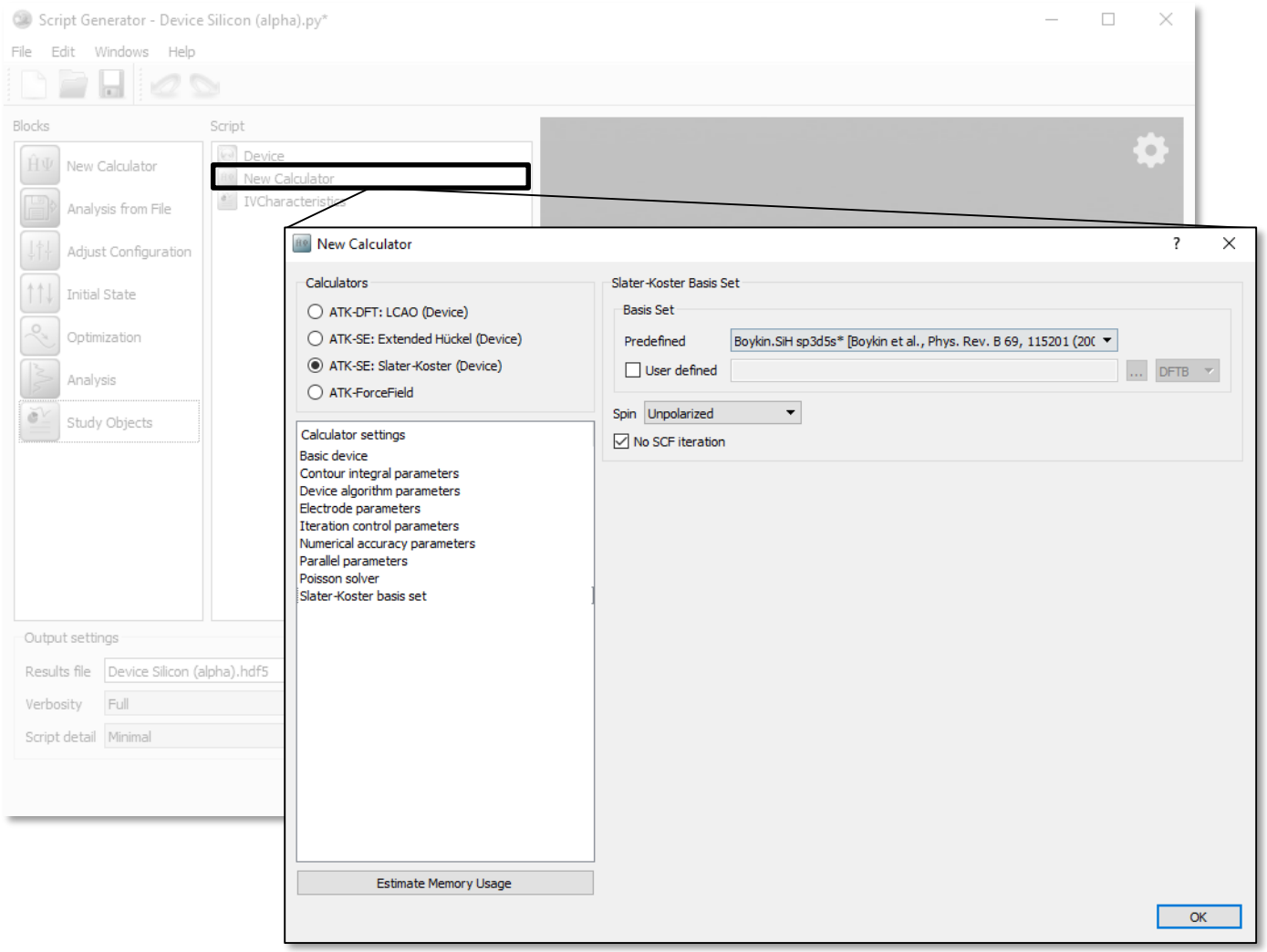
1 - Setting up the QuantumATK script.

The device configuration is send to the **Script Generator**, where the calculation script is created by adding:

- A new calculator block
- An **IVCharacteristics** block

In the new calculator block it is possible to set up the most appropriate calculator for the device of choice.

In the present example the ATK-SE: Slater-Koster (Device) calculator is used.



More info at: *docs.quantumwise.com/tutorials/ivcharacteristics/ivcharacteristics.html*

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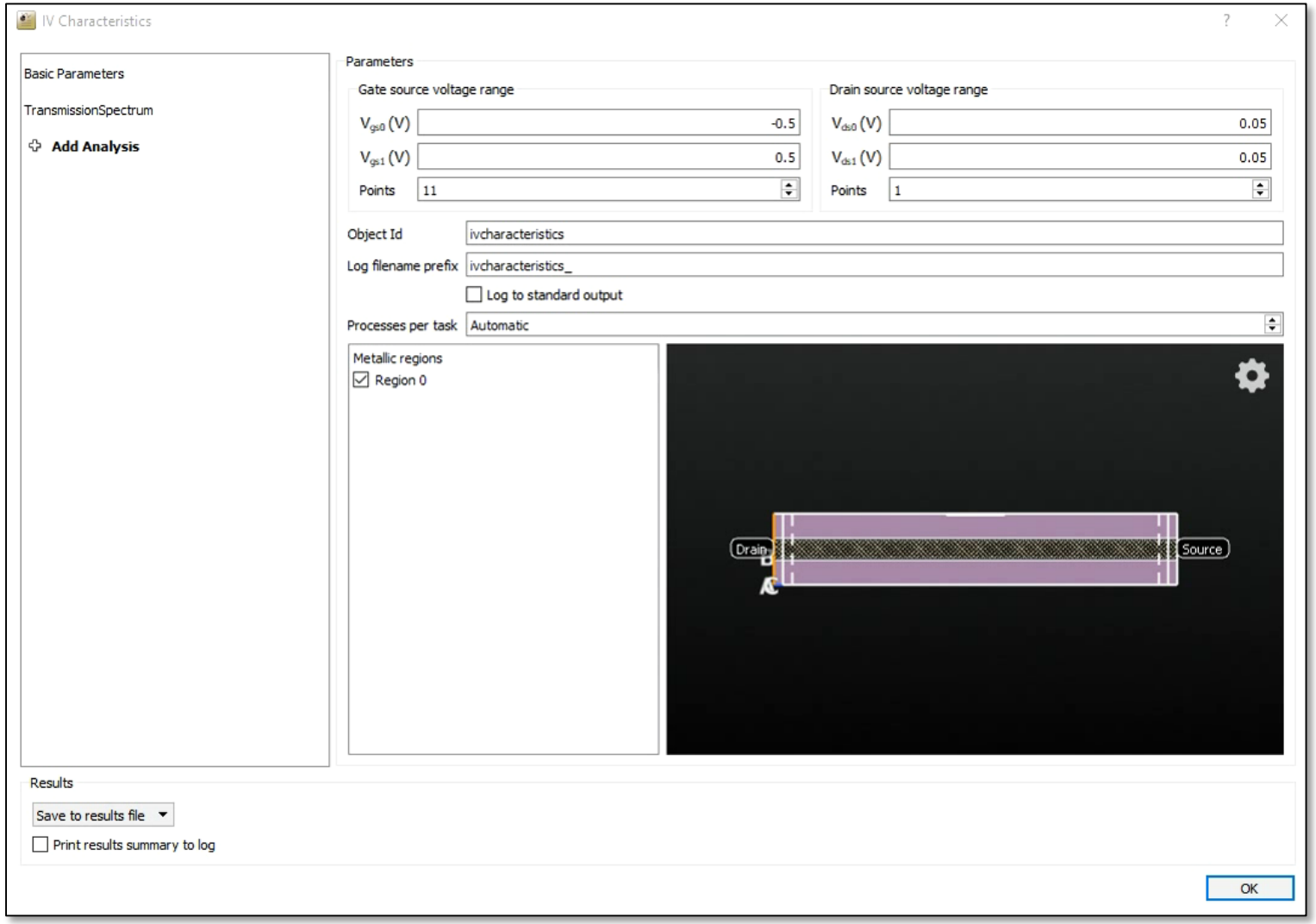
1.1 - A closer look at the IV Characteristics window…

The **IVCharacteristics window** is formed by three main sections which are used to:

1. Select the parameters of each part of the IVCharacteristics study object:
   - Basic Parameters
   - Transmission Spectrum analysis
   - Additional analyses for each data point.

2. Modify the parameters of each part of the Characteristics study object.

3. Edit the output options of the study object.



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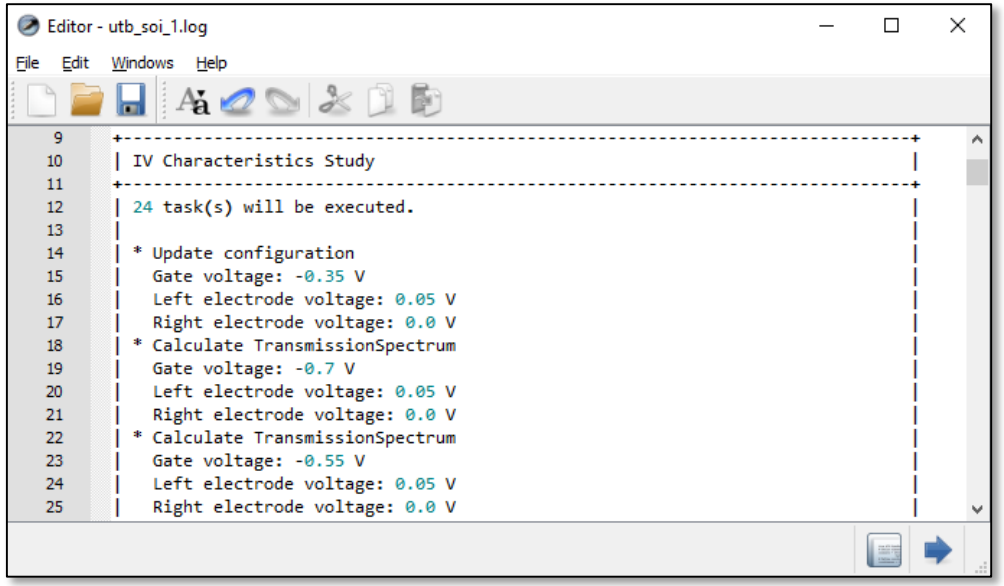
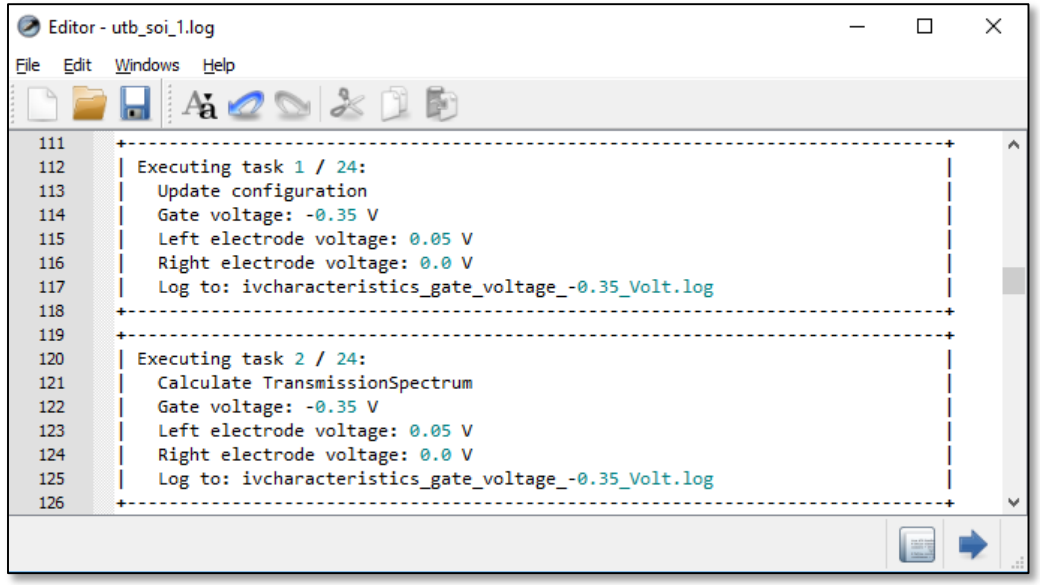
2 - Inspecting the log file.





A detailed summary of the tasks performed by the Study Object is printed out, indicating:

- The total number of tasks
- The step-by-step workflow

During execution of the workflow, an infobox is printed out for each of the executed tasks.

More info at: *docs.quantumwise.com/tutorials/ivcharacteristics/ivcharacteristics.html*

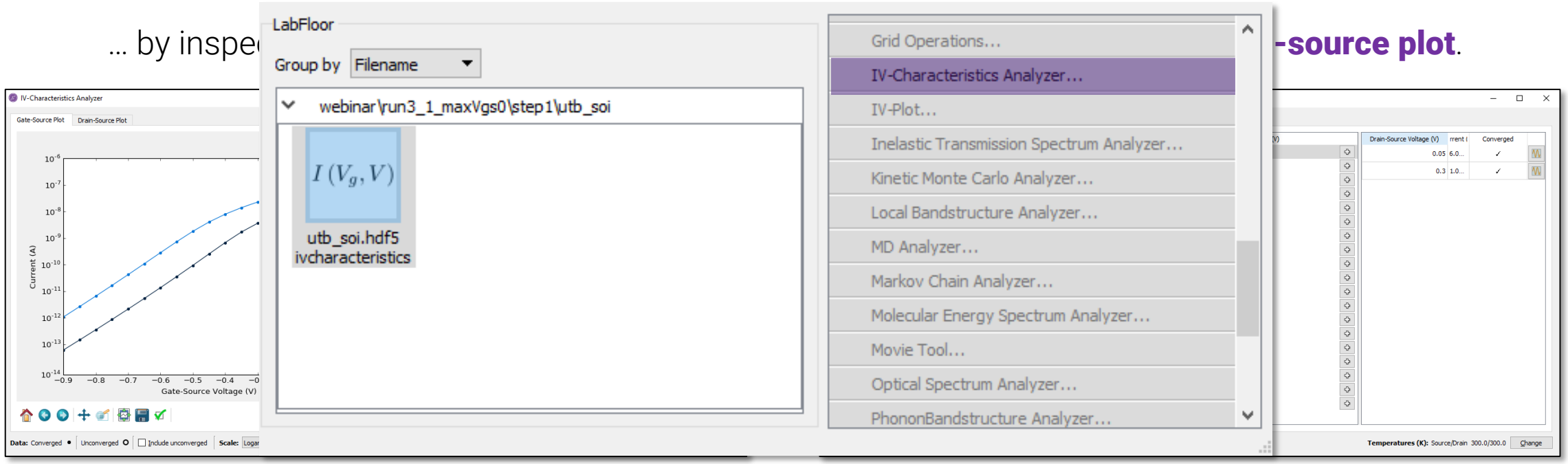
Analyzing the SOI device using the IV Characteristics study object.

1 - Analyzing the results using the IVCharacteristics analyzer…

2 - Extending the range of the data points.

Analyzing the results using the IVCharacteristics analyzer…

… by inspe -source plot.



More info at: *docs.quantumwise.com/tutorials/ivcharacteristics/ivcharacteristics.html*

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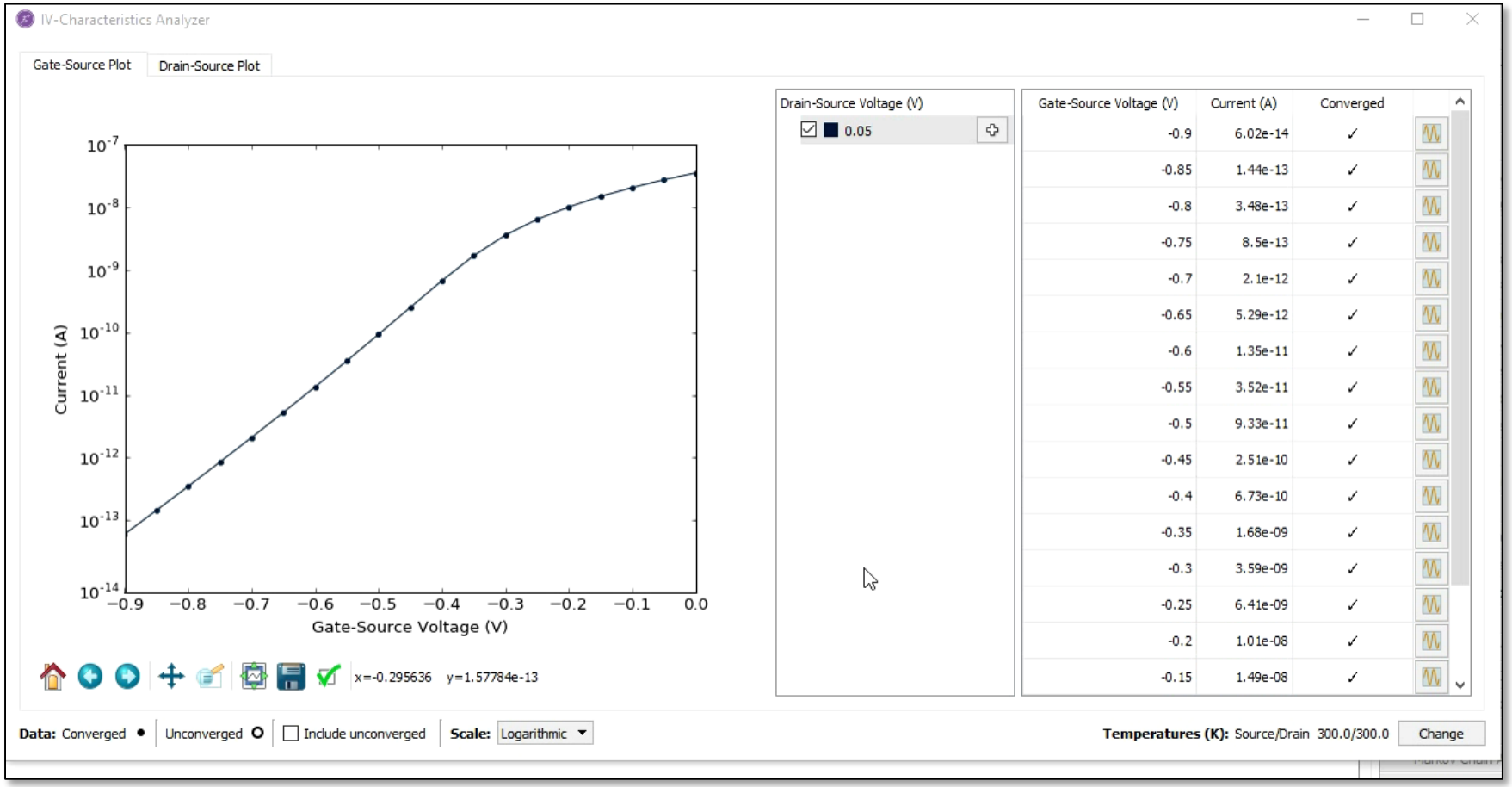
Analyzing the results using the IVCharacteristics analyzer…

In the **Gate-source plot** window it is possible to:

1. Check the convergence of the calculated data points.

2. Inspect the results and calculate electrical parameters such as:
   - On/Off ratio
   - Subthreshold slope
   - Transconductance

The calculated subthreshold slope of 123 mV/dec is in good agreement with that measured experimentally [1].



[1] S. Migita et al. Electrical performances of junctionless-FETs at the scaling limit (lch = 3 nm). *Proceedings of the Electron Device Meeting (IEDM) 2012*, 2012.

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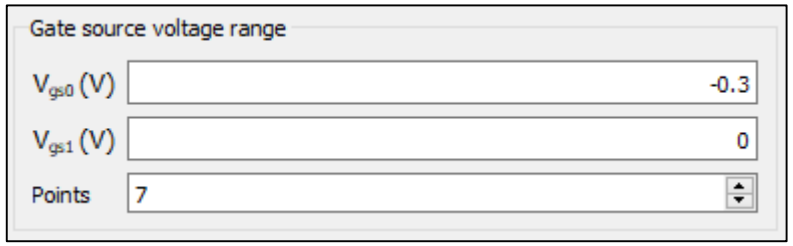
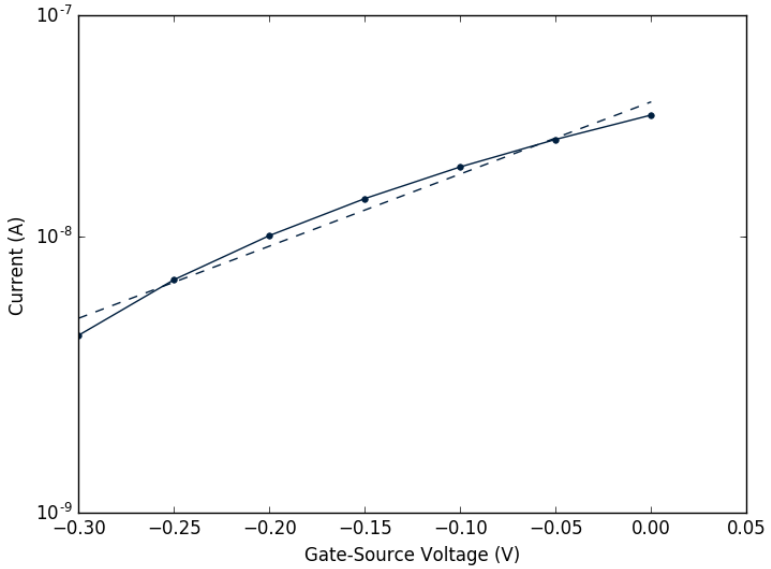
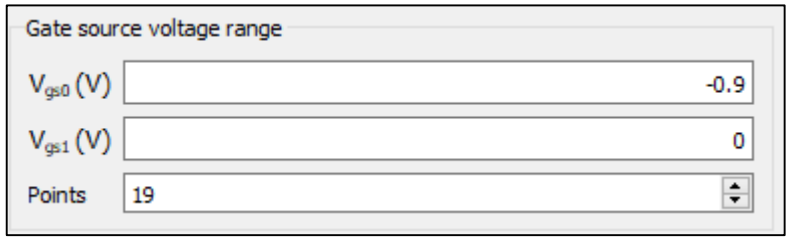
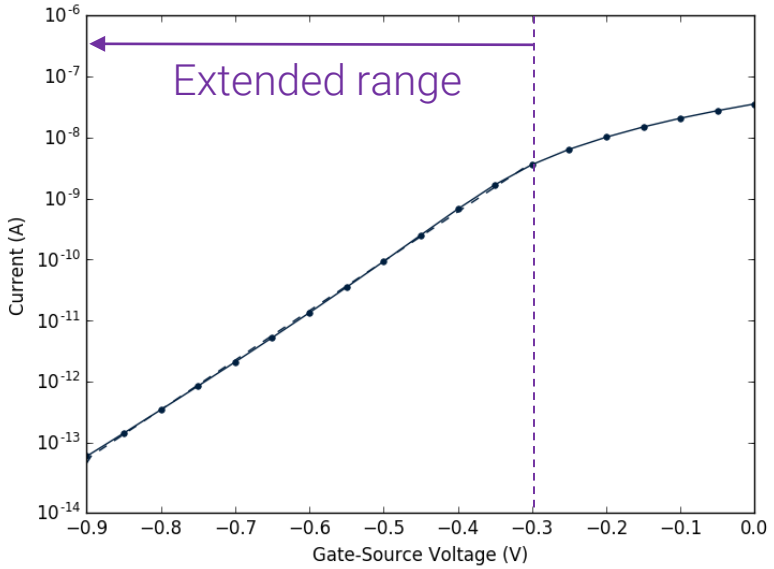
Extending the range of the data points.





Subthreshold slope = 307 mV/dec





Subthreshold slope = 123 mV/dec

- Additional data points can be added by simply extending the Gate source voltage range and re-running the script.
- The data points that are already present are not re-calculated.

More info at: *docs.quantumwise.com/tutorials/ivcharacteristics/ivcharacteristics.html*

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Conclusions

More information on **docs.quantumwise.com**:

Introduction to the Study Objects:
docs.quantumwise.com/manual/includes/Study.html

Tutorial: "Electrical characteristics of devices using the IVCharacteristics study object": *docs.quantumwise.com/tutorials/ivcharacteristics/ivcharacteristics.html*

Documentation of the IVCharacteristics study object:
docs.quantumwise.com/manual/Types/IVCharacteristics/IVCharacteristics.html

Thank you

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