In [1]:

```
%%capture
import pandas as pd
import matplotlib.pyplot as plt
import matplotlib.gridspec as gridspec
%matplotlib inline
plt.style.use('seaborn-v0_8-whitegrid')
from matplotlib.legend_handler import HandlerTuple
import matplotlib.ticker as ticker
!pip freeze > requirements.txt
!pip freeze | grep -v -f requirements.txt - | grep -v '^#' | grep -v '^-e ' | xargs pip uninstall -y
```

Abstract

This carrier quantum-confinement simulation of Silicon (Si) inversion layer, pertains to a 1D MOS Capacitor at 300K, using COMSOL's '**Multiphysics®**' and nanoHUB's '**Schred** 1.0' tool. Such a simulation requires calculating the carrier concentration (in this case electron) as a function of vertical distance from the oxide-channel interface (referred to as 'Arc length' in the upcoming plots), based on standard MOS device parameters (referred from **[1] COMSOL Documentation**) and carrier transport formalisms such as -

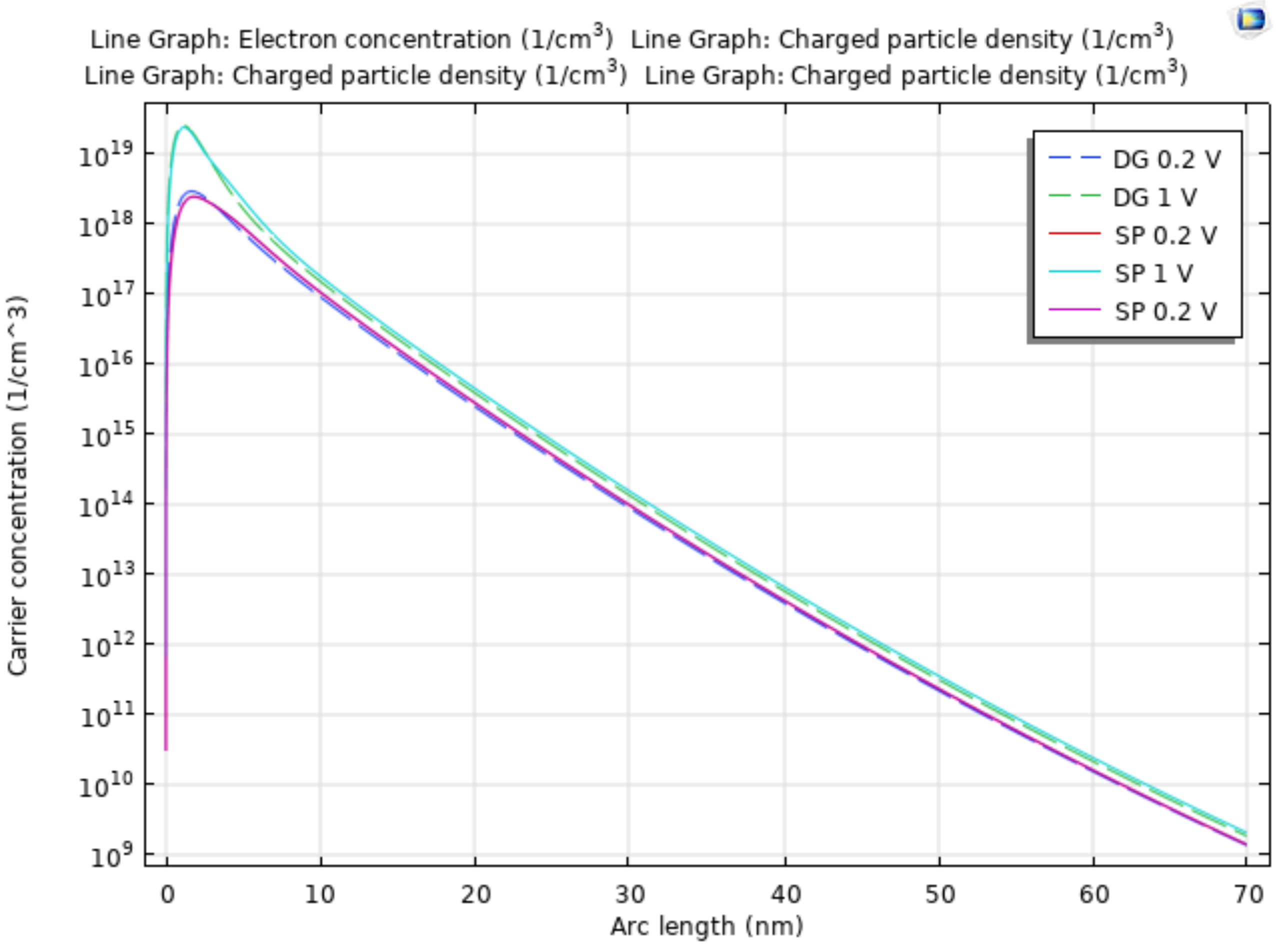
1. Density Gradient: based on a quantum potential-corrected continuum transport description of carriers, as originally formulated in **[2]**.
2. Schrödinger-Poisson: based on a full quantum transport description of carriers using non-equilibrium Greene's function, as originally formulated in **[3]**.

Table of Contents

- **Part I: Density-Gradient and Schrödinger-Poisson solution of inversion layer, using COMSOL**
  - **Simulations at $V_g = 0.2V, 1V$**
    - **Summary**
- **Part II: Schrödinger-Poisson solution of inversion layer, using NanoHUB and COMSOL**
  - **Simulations at $V_g = 1V$**
    - **Summary**
- **Part III: Classical-Poisson solution of inversion layer, using NanoHUB and COMSOL**
  - **Simulations at $V_g = 1V$ (in NanoHUB) and $V_g = 0.2V, 1V$ (in COMSOL)**
    - **Summary**
- **References**

Part I: Density-Gradient and Schrödinger-Poisson solution of inversion layer, using COMSOL

Simulations at $V_g = 0.2V, 1V$



	Density-Gradient solution (V_g = 0.2V, 1V)	Schrödinger-Poisson solution (V_g = 0.2V)	Schrödinger-Poisson solution (V_g = 1V)
Time elapsed (s)	9	72	101
Memory usage (GB)	1.01	1.09	1.27

Summary

1. As noted in the table above (and as mentioned in [2]), the Density-Gradient formulation is more computationally efficient than Schrödinger-Poisson formulation in solving carrier concentrations (and with similar solutions w.r.t that of Schrödinger-Poisson formulation $\forall V_g$, as observed in the plot above) across the vertical Si channel.
2. Both formulations capture the effect of electron quantum-confinement near 3-4 nm range $\forall V_g$ (observed as peaks in the plot above). This effect is due to -
   - Electron quantisation in the Si channel stemming from a degenerate Si bandstructure.
   - Increasing potential barrier height at the oxide-channel interface due to ever decreasing oxide thickness (which has to do with MOS process node scale-down), leading to zero probability of electron tunneling into the oxide.

Part II: Schrödinger-Poisson solution of inversion layer, using NanoHUB and COMSOL

Simulations at $V_g = 1V$

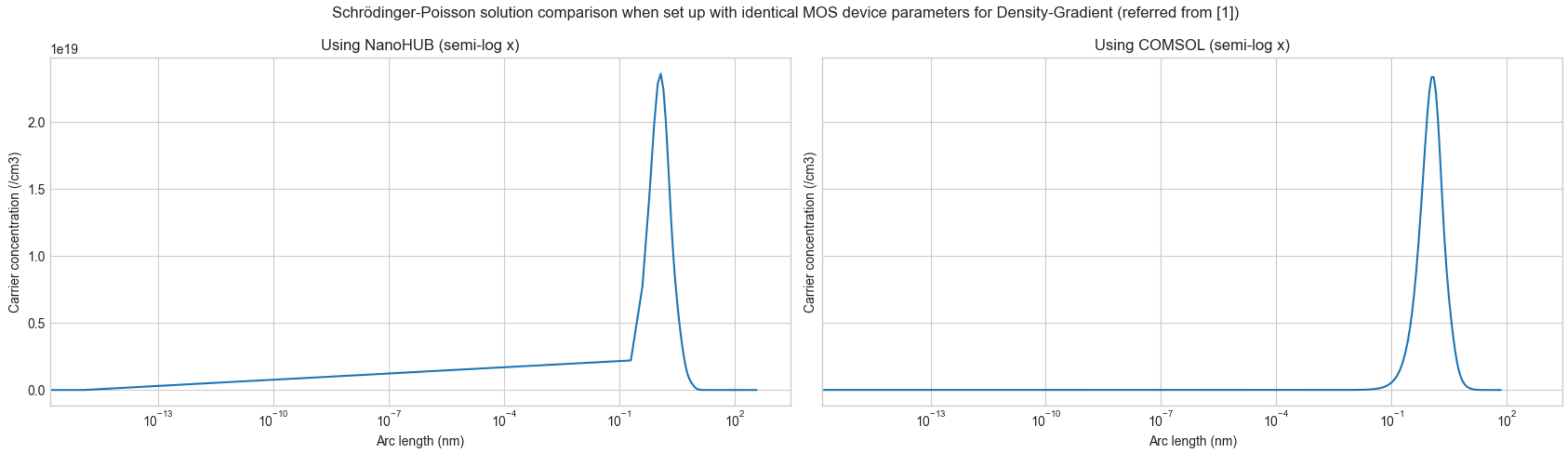
In [2]:

```
SPNanoHUB = pd.read_csv('Part II/3.txt', skiprows=4, nrows=999, header=None)
SPCOMSOL = pd.read_fwf('Part I/2.txt', skiprows=8, nrows=199, header=None)
fig,axes = plt.subplots(nrows=1,ncols=2,tight_layout=True,sharex=True,sharey=True,figsize=(17, 5))
fig.suptitle('Schrödinger-Poisson solution comparison when set up with identical MOS device parameters for Density

plt.subplot(121)
plt.plot(SPNanoHUB[0],SPNanoHUB[1])
plt.xscale('log')
axes[0].set_xlabel('Arc length (nm)')
axes[0].set_ylabel('Carrier concentration (/cm3)')
axes[0].set_title('Using NanoHUB (semi-log x)')

plt.subplot(122)
plt.plot(SPCOMSOL[0],SPCOMSOL[1])
plt.xscale('log')
axes[1].set_xlabel('Arc length (nm)')
axes[1].set_ylabel('Carrier concentration (/cm3)')
axes[1].set_title('Using COMSOL (semi-log x)')
```

```
Out[2]: Text(0.5, 1.0, 'Using COMSOL (semi-log x)')
```



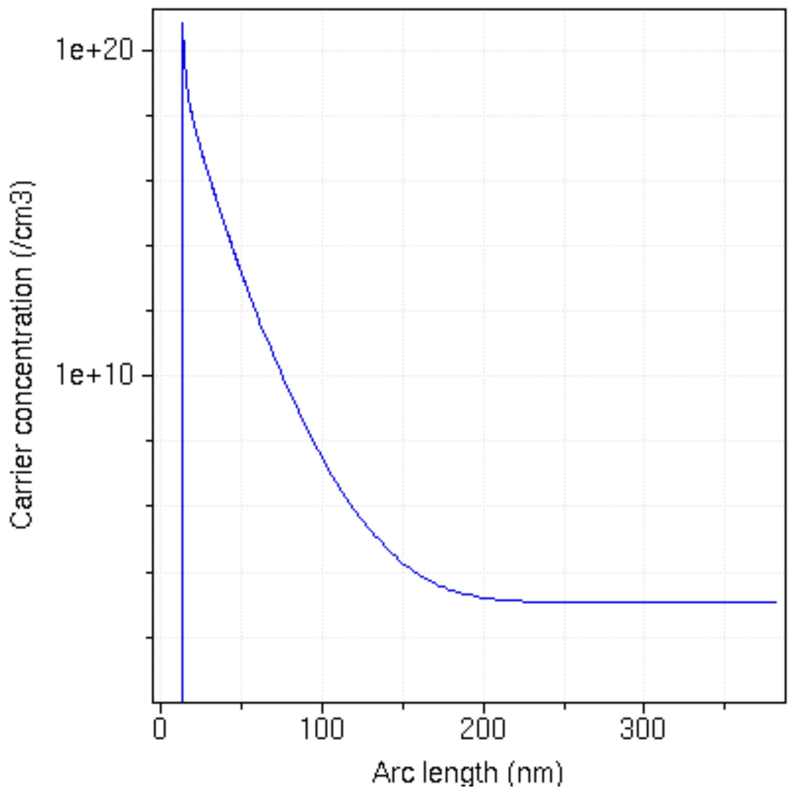
Summary

1. Both NanoHUB (Schred tool) and COMSOL capture the electron charge centroid (peaks in the plots above) at the same position in the vertical Si channel, which indicates that the Schrödinger-Poisson formulation in both tools are similarly defined.
2. The slight discreteness in the NanoHUB plot above indicates a lack of enough discretisation nodes defined along the vertical Si channel in the Schred tool.

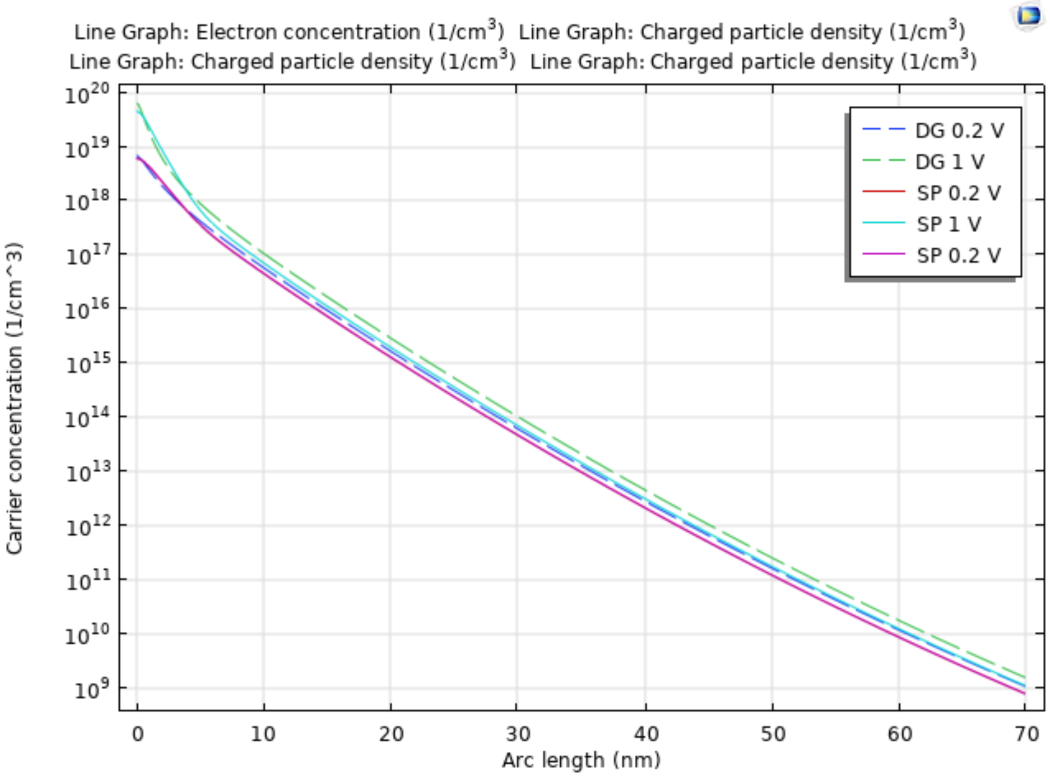
Part III: Classical-Poisson solution of inversion layer, using NanoHUB and COMSOL

Simulations at $V_g = 1V$ (in NanoHUB) and $V_g = 0.2V, 1V$ (in COMSOL)

Using NanoHUB



Using COMSOL



Summary

1. To perform a Classical-Poisson simulation of the inversion layer:
   - Using NanoHUB Schred: As noted in page 11 of **[4]**, Schred 2.0 with the semiclassical charge model is used and the resulting simulation plot is shown in the left above.
   - Using COMSOL: As inferred from **[1]** and based on the discussion in point 2 of Summary in Part I) -
     A. For classical approximation from Density-Gradient formulation: electron mass (meDG) is set to 10xme_const/3 (inferred from page 7 of **[1]**), and n barrier height at oxide interface (Φ_n^{Ox}) is set to 0 (inferred from page 8 of **[1]**).
     B. For classical approximation from Schrödinger-Poisson formulation: Zero Probability node in the COMSOL model tree is disabled (inferred from page 13 of **[1]**).
     C. The combined resulting simulation plot (classical approximation from Density-Gradient \& Schrödinger-Poisson formulations) is shown in the right above.
2. Both plots above (Classical-Poisson simulations using NanoHUB and COMSOL) indicate a monotonically decreasing inversion electron concentration from the oxide-Si channel interface (non-existent electron charge centroids at further depths in the vertical Si channel), which is the case when there is no carrier quantum-confinement effect.

References

- [1] **COMSOL Documentation - Density-Gradient and Schrödinger–Poisson Results for a Silicon Inversion Layer**
- [2] **Density-gradient theory: a macroscopic approach to quantum confinement and tunneling in semiconductor devices - M.G. Ancona**
- [3] **Nanoscale device modeling: the Green's function method - Supriyo Datta**
- [4] **Schred Documentation - Quantum Size Effects and the Need for Schred - Dragica Vasileska**

Additional information

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Data and config file at: Github