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Department of Mechanical and Process Engineering

Green's Function Approach to Efficient 3D Electrostatics of Multi-Scale Problems

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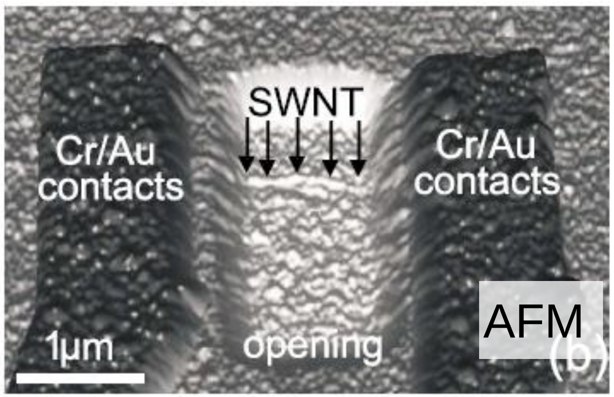
Micro and Nanosystems
Department of Mechanical and Process Engineering

BRNC | FIRST

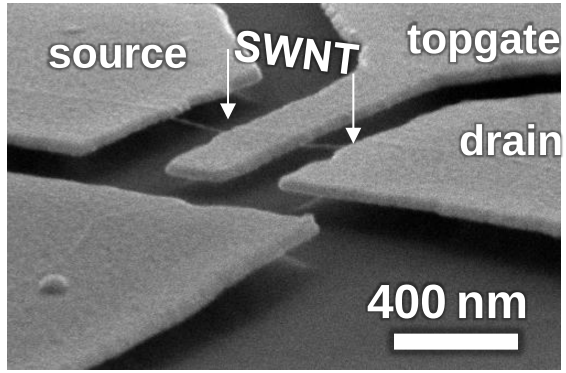
COMSOL CONFERENCE
2017 ROTTERDAM

Carbon nanotube transducers



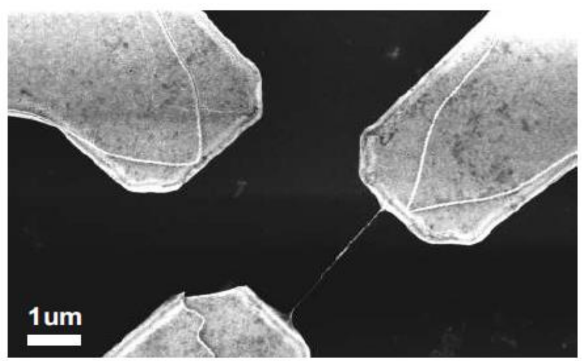
chemical sensors

M. Mattmann *et al.*,
Appl. Phys. Lett. 94, 183502 (2009)



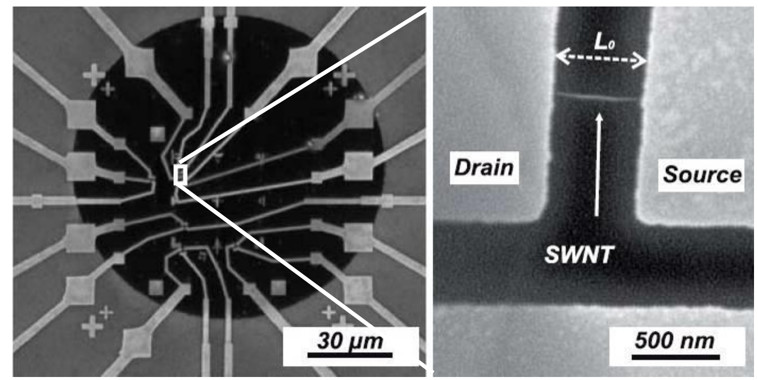
displacement sensor, suspended quantum dots

C. Stampfer *et al.*,
Nano Lett. 6, 1449 (2006)
R. Leturcq *et al.*,
Nature Phys. 5, 327 (2009)



tunable resonators

S.-W. Lee, IEEE NEMS, 2011

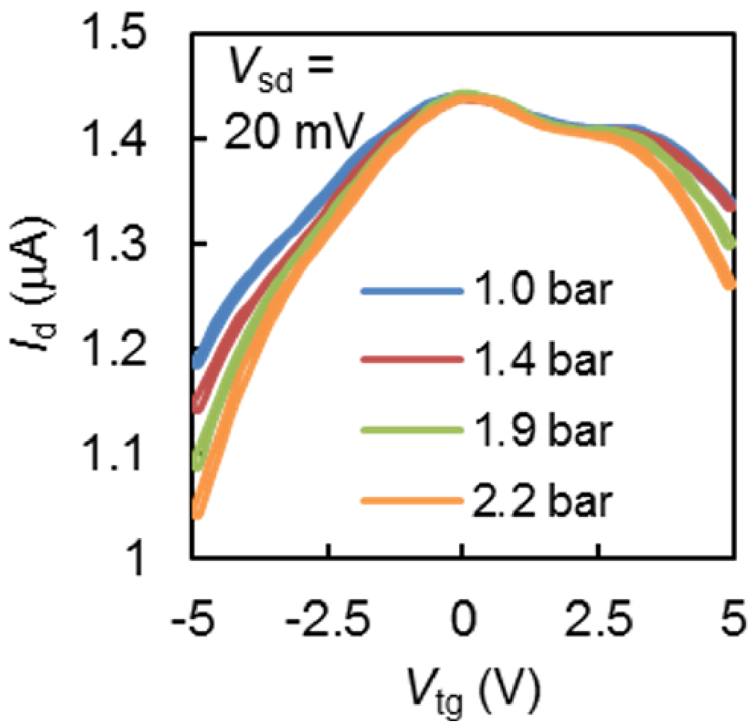


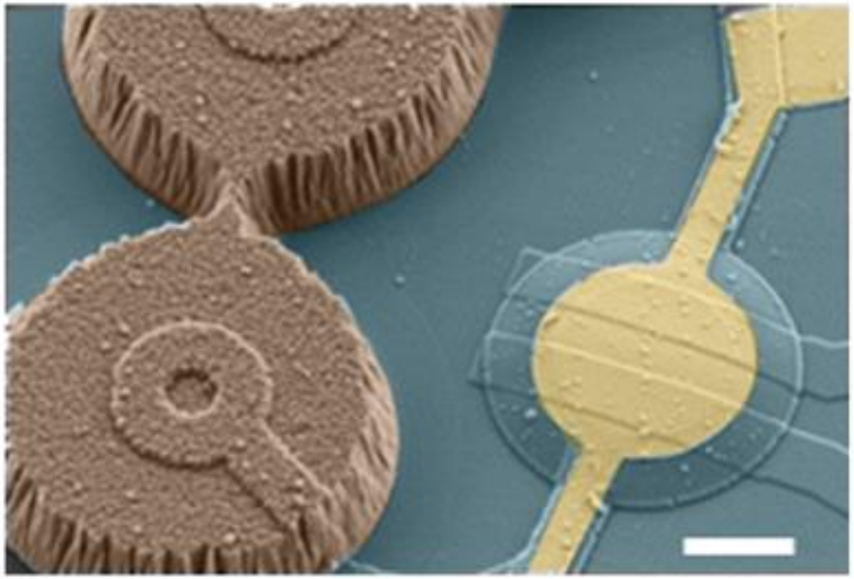
pressor sensors

T. Helbling *et al.*,
Transd.'07&E. XXI, 2, 2553 (2007)

T. Helbling *et al.*,
Proc. IEEE MEMS 2009, 575 (2009)

Open research questions

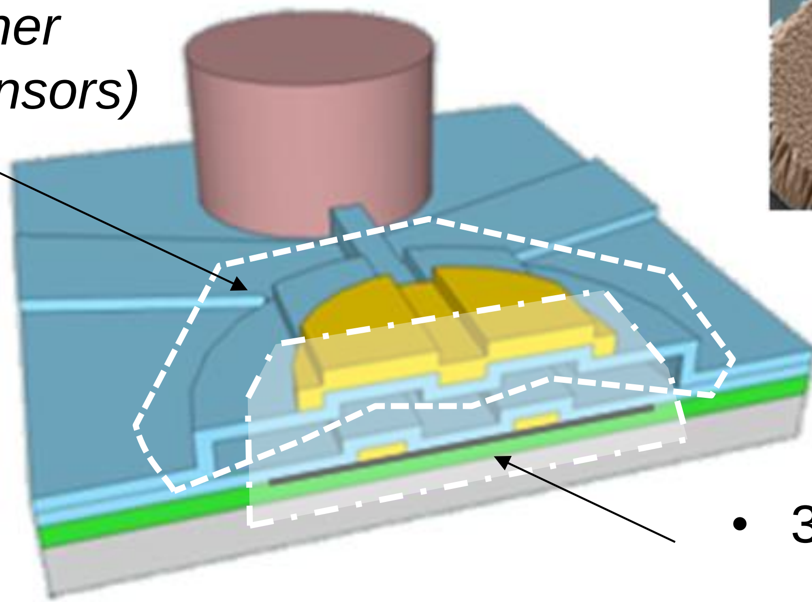


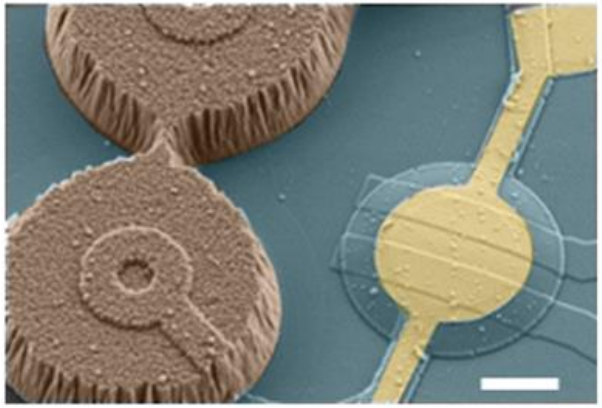


To improve our understanding and to design better sensors,
we need a simulation platform able to model all relevant physics!

Relevant physics

- 3D mechanics of thin film membranes with topography
- thermal stresses
- *(other physics for other sensors, e.g. gas sensors)*





- 3D field effect transistor
  - electrostatics
  - charge transport

We chose COMSOL for the ability to model these and much more (open to other sensors)

Modeling a 3D carbon nanotube FET

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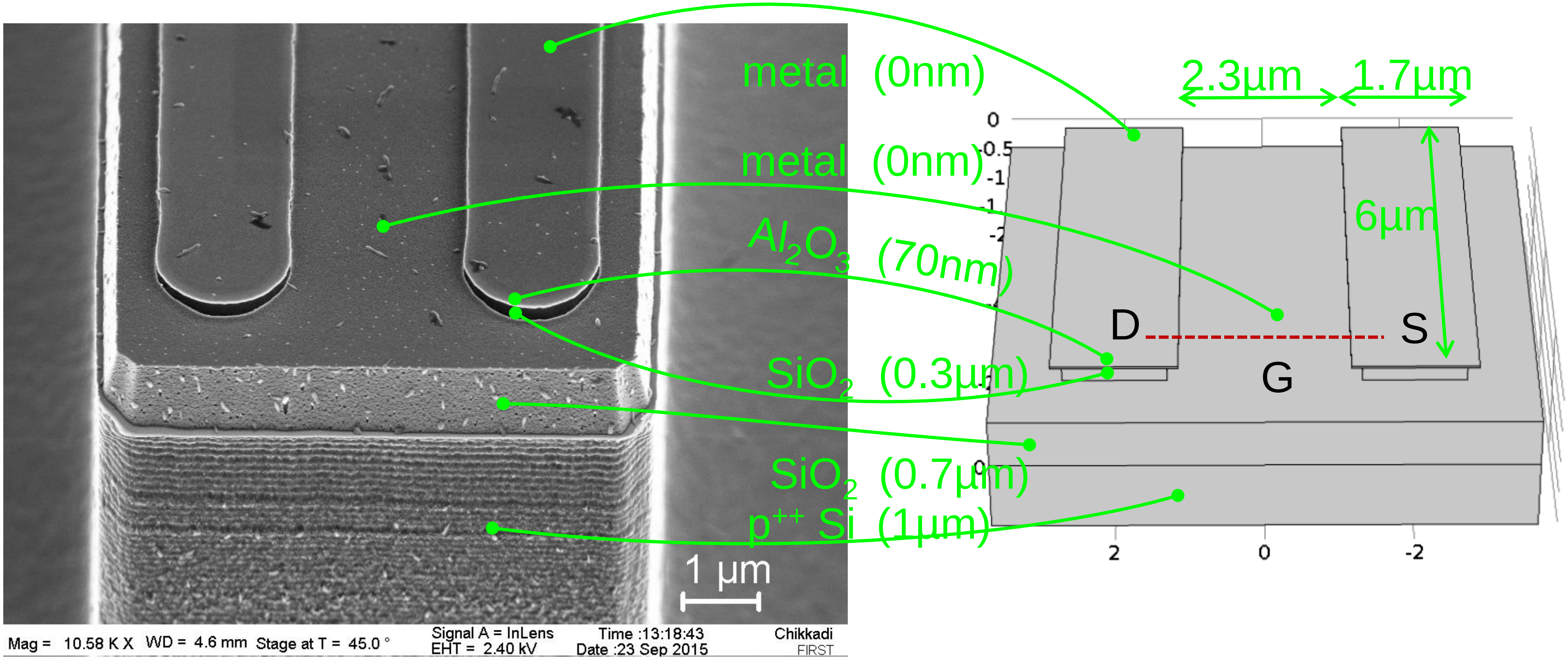
Benchmark model



How is the I-V characteristic of such a device computed?

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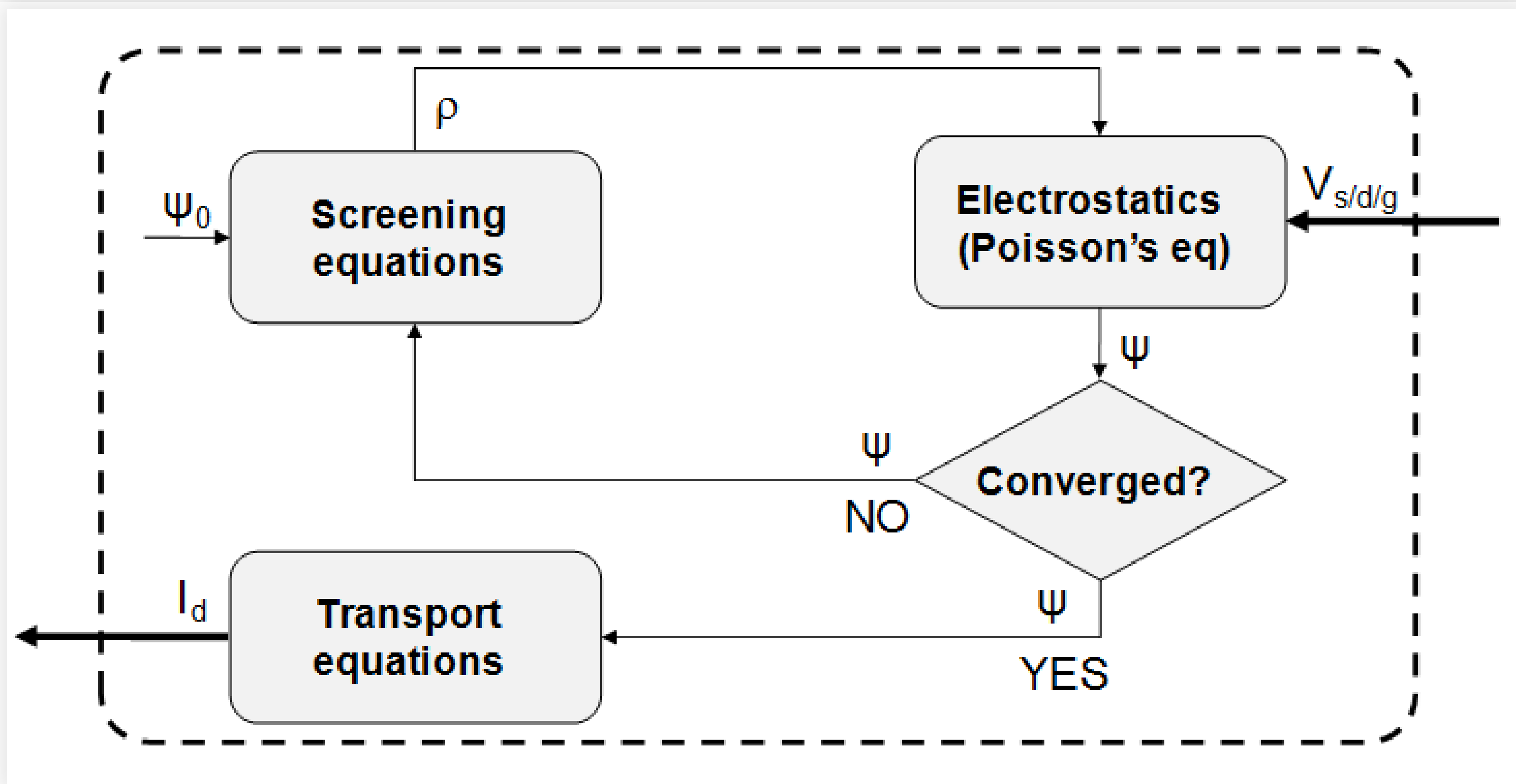
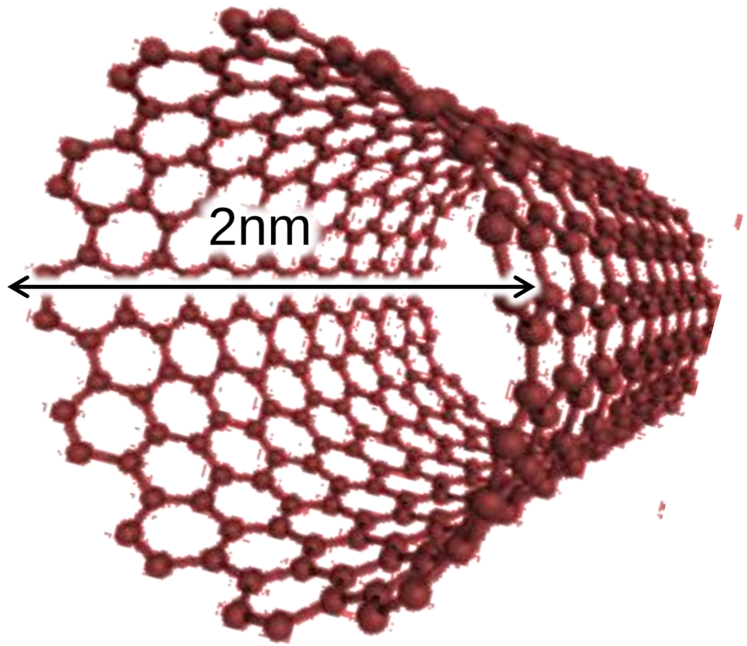
The self-consistent procedure

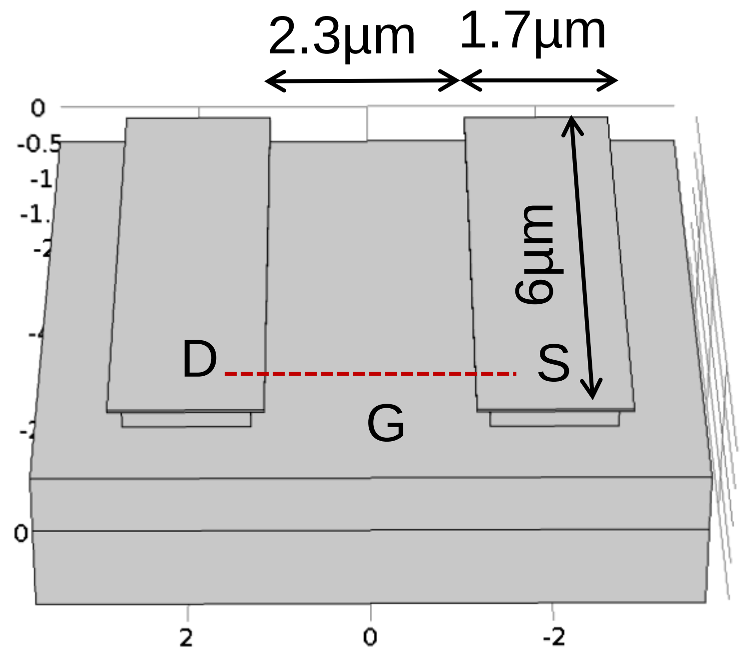


- Iterate between screening eqs. (Schrödinger) and Poisson eqs. till potential convergences
- After convergence, solve transport eqs.

The challenge

The challenge/bottleneck is iterating over the 3D Poisson equation (1’000-10’000 iterations needed for an I-V characteristic)





The scale range is from 1Å to 10µm (5 orders) and geometry is 3D!

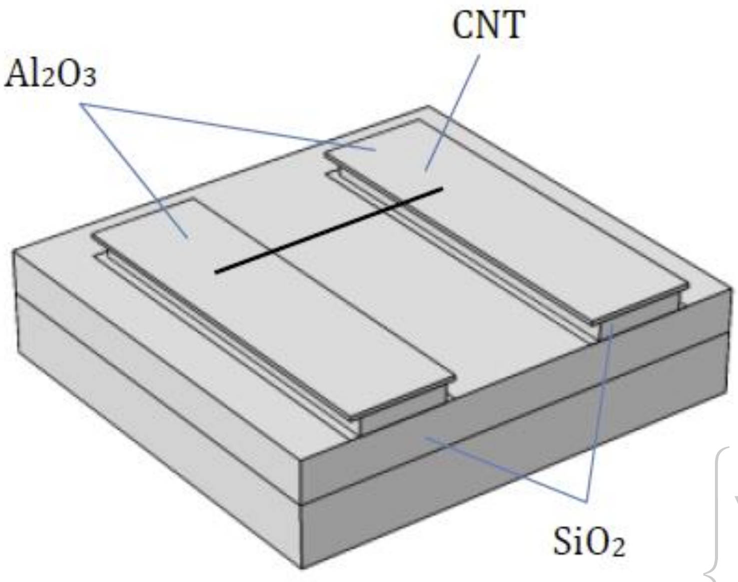
The solution

The challenge/bottleneck is iterating over the 3D Poisson equation (1’000-10’000 iterations needed for an I-V characteristic)

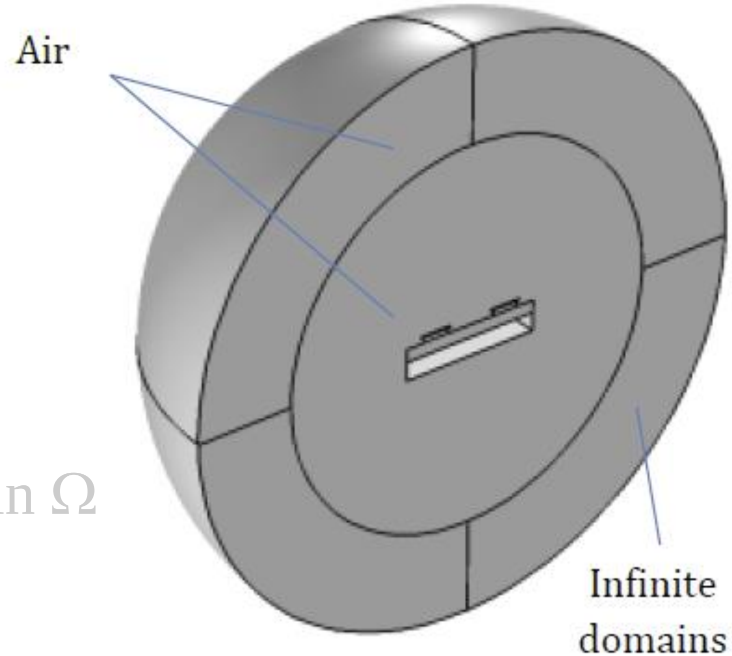
The solution is:

- compute elementary solutions from which an arbitrary solution can be obtained as a (cheap) combination
- accelerate (or approximate) the computation of each elementary solution

Breakdown into elementary solutions



$$\begin{cases} \nabla^2 \psi(\mathbf{r}) = -\dfrac{\rho(\mathbf{r})}{\varepsilon(\mathbf{r})} \text{ in } \Omega \\ \psi = V_{s|d|g} \text{ at } \delta\Omega \end{cases}$$



$$3\times \begin{cases} \nabla^2 \psi(\mathbf{r}) = 0 \text{ in } \Omega \\ \psi = 1\text{ V at } \delta\Omega_s \\ \psi = 0\text{ V at } \delta\Omega_{\mathrm{d,g}} \end{cases}$$

(Laplace problem)

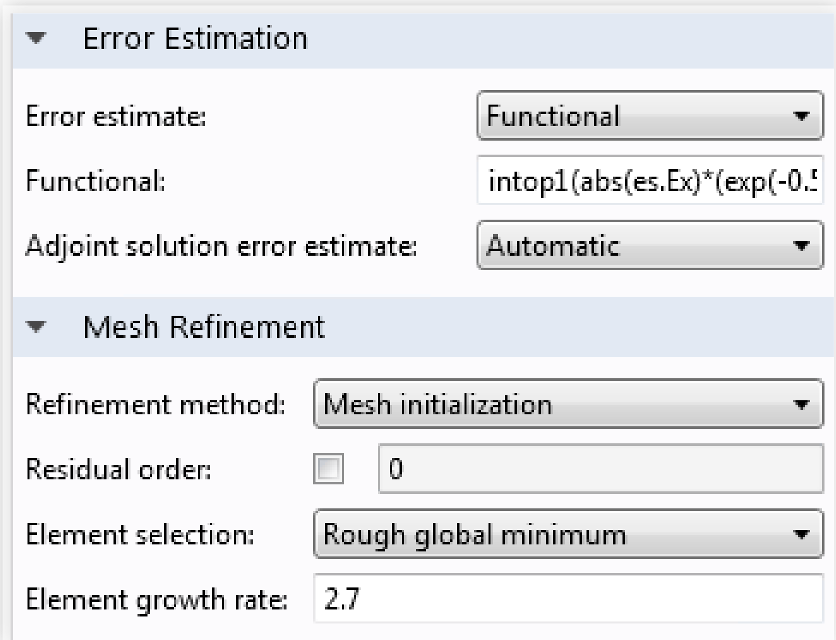
$$N\times \begin{cases} \nabla^2 \psi(\mathbf{r}) = -\dfrac{\delta(\mathbf{r}-\mathbf{r}_0)}{\varepsilon(\mathbf{r})} \text{ in } \Omega \\ \psi = 0 \text{ at } \delta\Omega \end{cases}$$

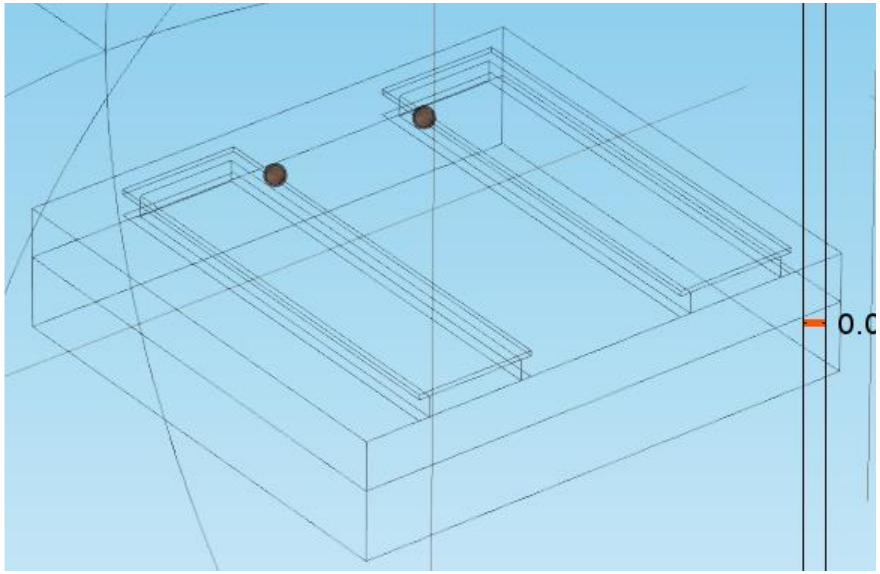
(Poisson Green's Functions)

Local adaptive mesh refinements

Key trick to accelerate the Laplace problem: Local adaptive mesh refinements, because we only care about the potential at contacts!

$$\int d^3\mathbf{r} \cdot |E_x(\mathbf{r})| \cdot \left[\exp\left(-\frac{|\mathbf{r}-\mathbf{r}_S|^2}{2\cdot\sigma^2} \right) + \exp\left(-\frac{|\mathbf{r}-\mathbf{r}_D|^2}{2\cdot\sigma^2} \right) \right]$$



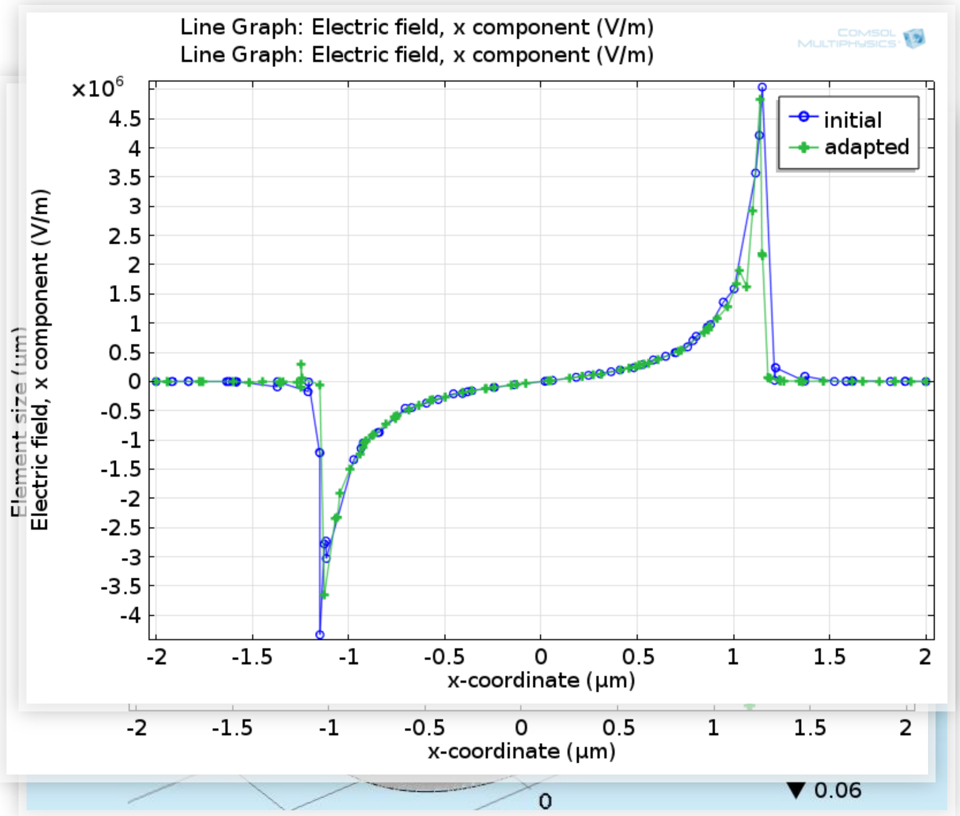


https://www.comsol.com/blogs/using-adaptive-meshing-local-solution-improvement/ Walter Frei | December 27, 2013

Adaptive mesh refinement comparison

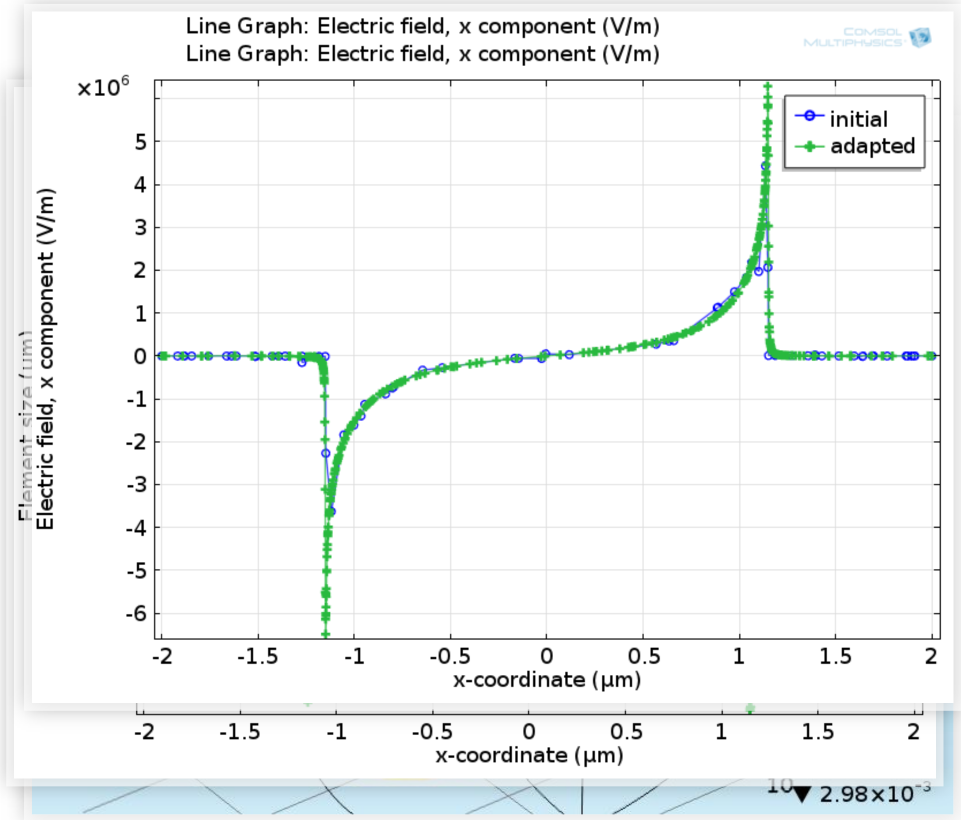
L2 Norm (Global refinement)

Number of DoF solved for: 139’020 ... 1’651’281.
Solution time: 259 s. (4 minutes, 19 seconds)



Functional (Local refinement)

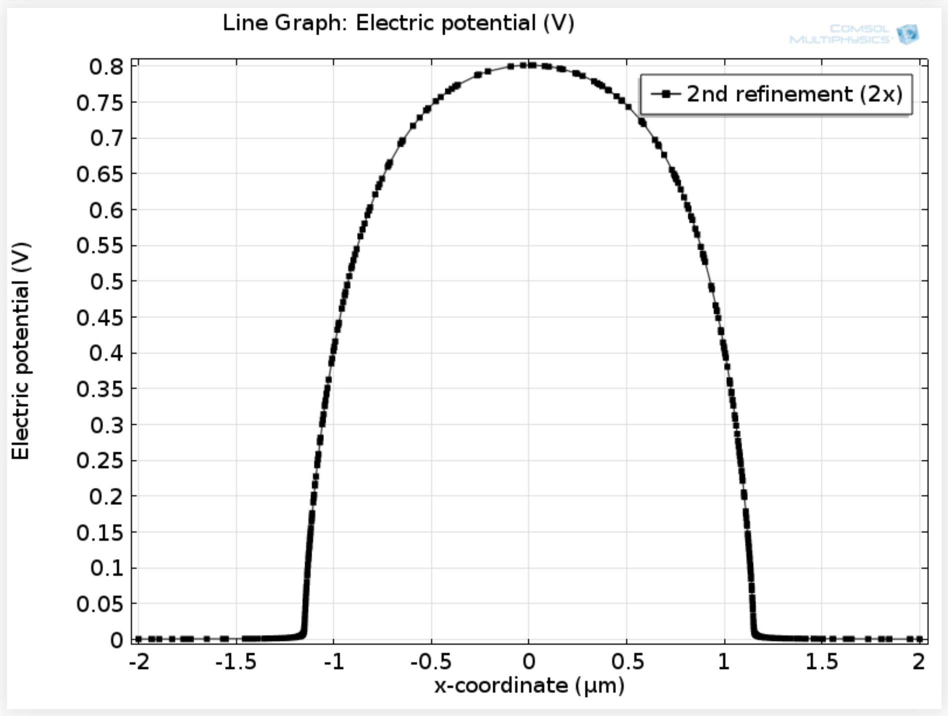
Number of DoF solved for: 42’031 … 158’820.
Solution time: 57 s.



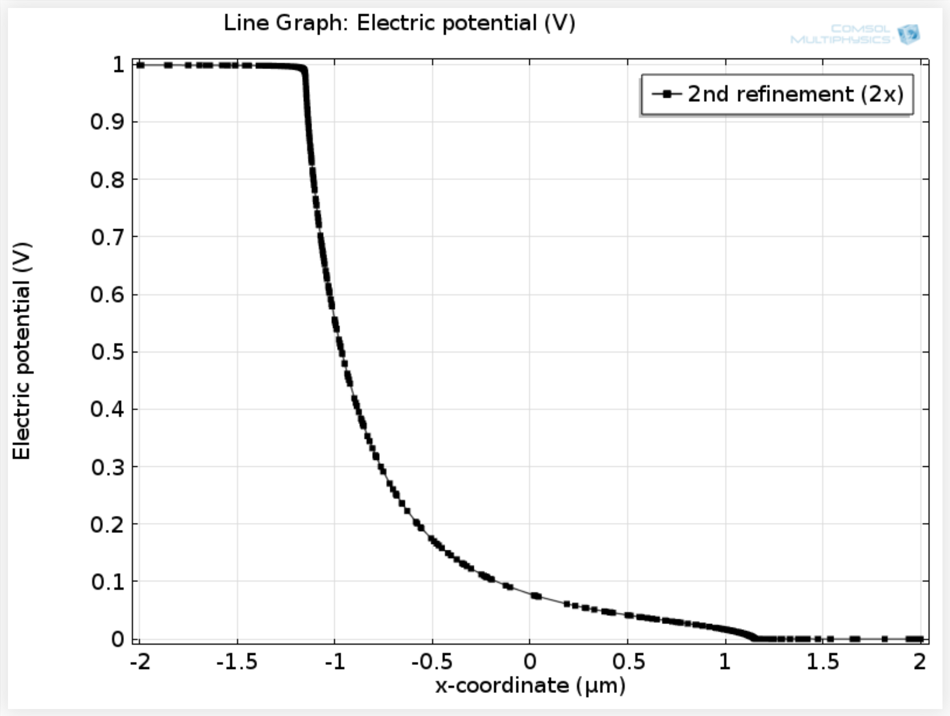
5-10× improvement over global mesh refinement!

Laplace problem: summary

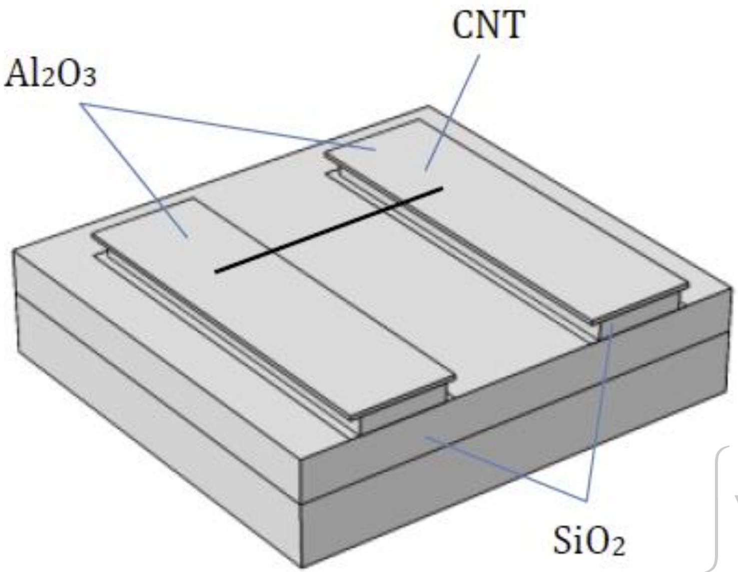
Gate response



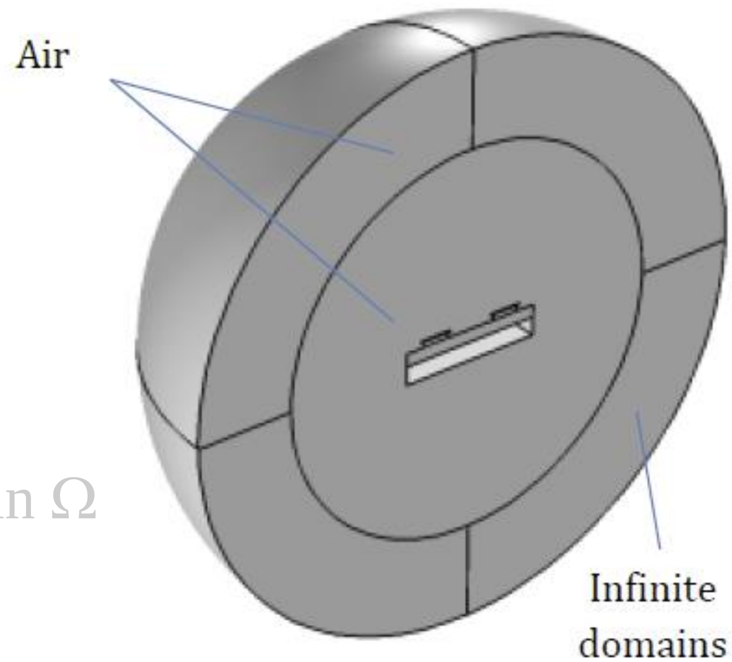
Source | Drain response



Breakdown into elementary solutions



$$\begin{cases} \nabla^2 \psi(\mathbf{r}) = -\dfrac{\rho(\mathbf{r})}{\varepsilon(\mathbf{r})} \text{ in } \Omega \\ \psi = V_{s|d|g} \text{ at } \delta\Omega \end{cases}$$



$$3\times \begin{cases} \nabla^2 \psi(\mathbf{r}) = 0 \text{ in } \Omega \\ \psi = 1\,\mathrm{V} \text{ at } \delta\Omega_s \\ \psi = 0\,\mathrm{V} \text{ at } \delta\Omega_{d,g} \end{cases}$$

(Laplace problem)

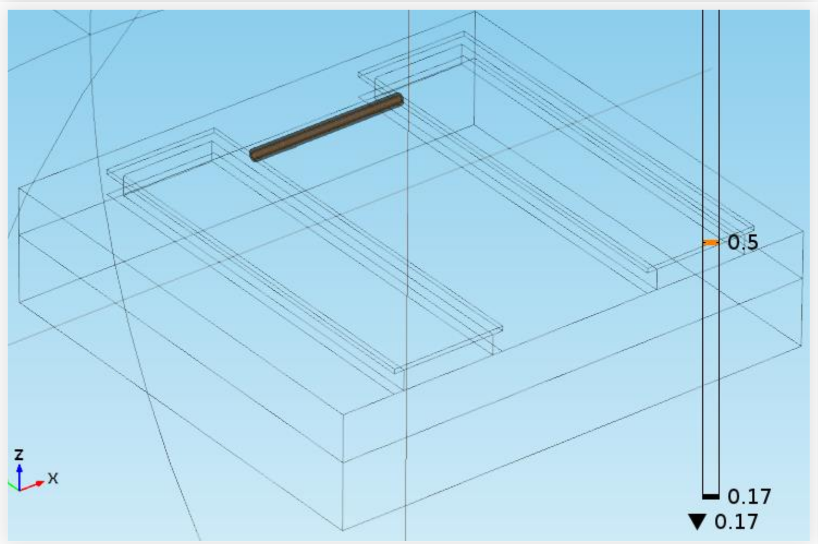
$$N\times \begin{cases} \nabla^2 \psi(\mathbf{r}) = -\dfrac{\delta(\mathbf{r}-\mathbf{r}_0)}{\varepsilon(\mathbf{r})} \text{ in } \Omega \\ \psi = 0 \text{ at } \delta\Omega \end{cases}$$

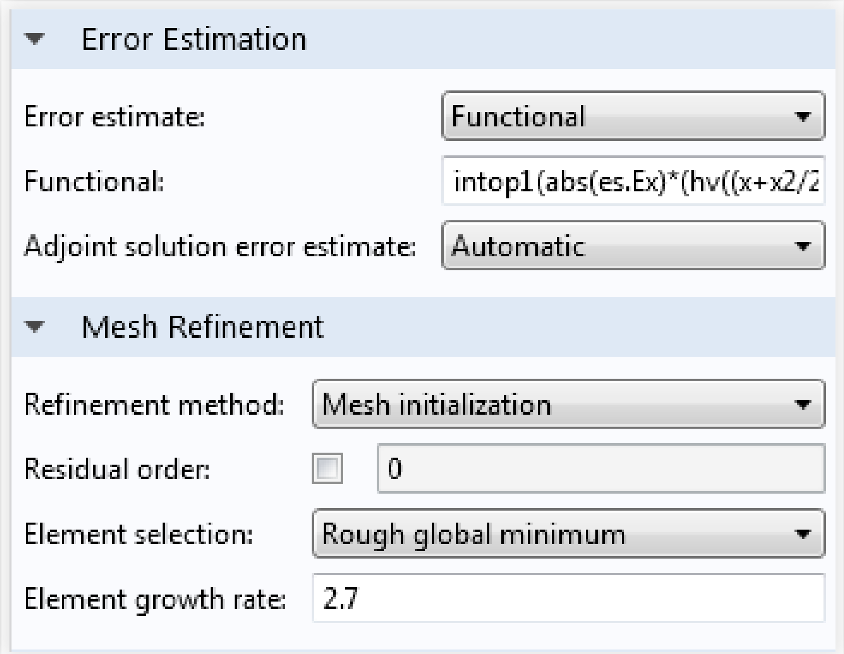
(Poisson Green's Functions)

Local adaptive mesh refinements

Key trick to accelerate the Poisson GF problem: Local adaptive mesh refinements plus an interpolation scheme to skip redundant computations

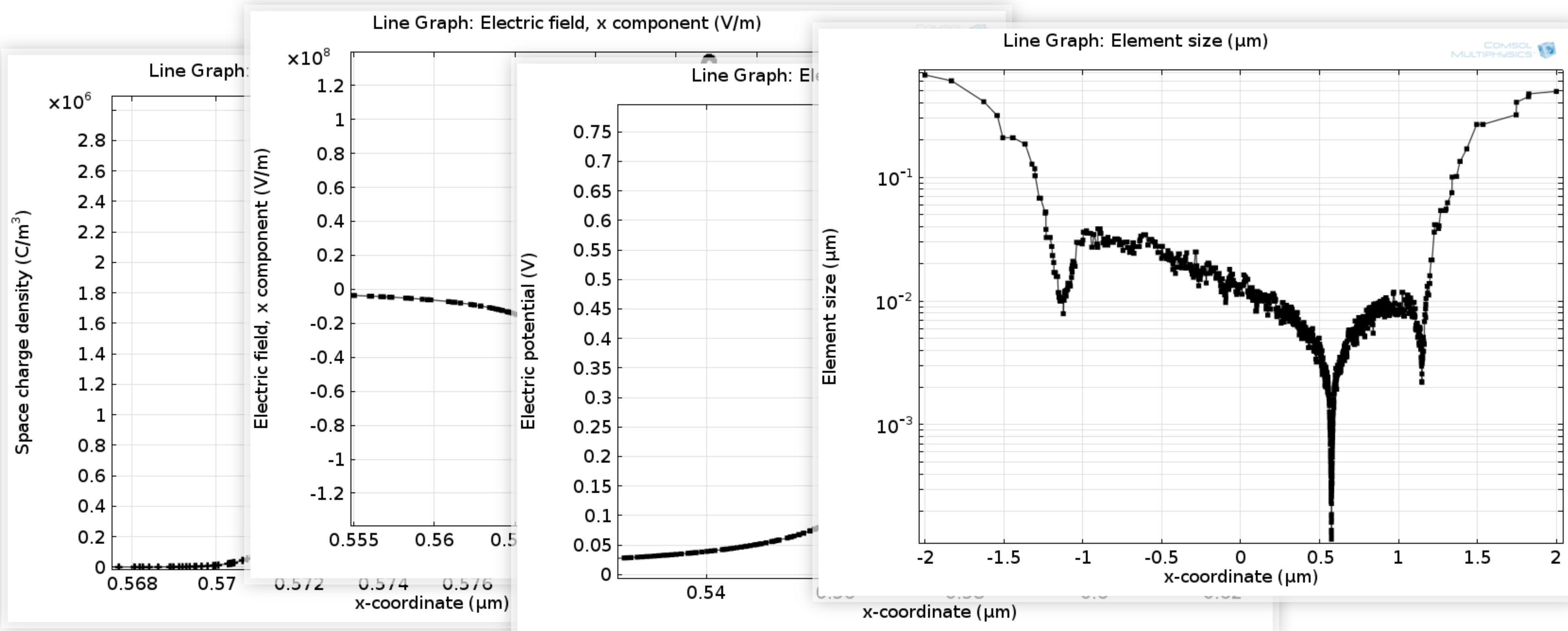
$$\int d^3\mathbf{r} \cdot |\mathrm{E}_x(\mathbf{r})| \cdot \frac{1}{2}\left[\tanh\left(\frac{x - x_S + 30\mathrm{nm}}{10\mathrm{nm}}\right) - \tanh\left(\frac{x - x_D - 30\mathrm{nm}}{10\mathrm{nm}}\right)\right] \cdot \exp\left(-\frac{(y - y_{NT})^2 + (z - z_{NT})^2}{2 \cdot r_{NT}^2}\right)$$





Poisson GF sub-problem: summary

“Point” (Gaussian) probe charge at x/L=0.76



1Å spatial resolution reached at the charge site!

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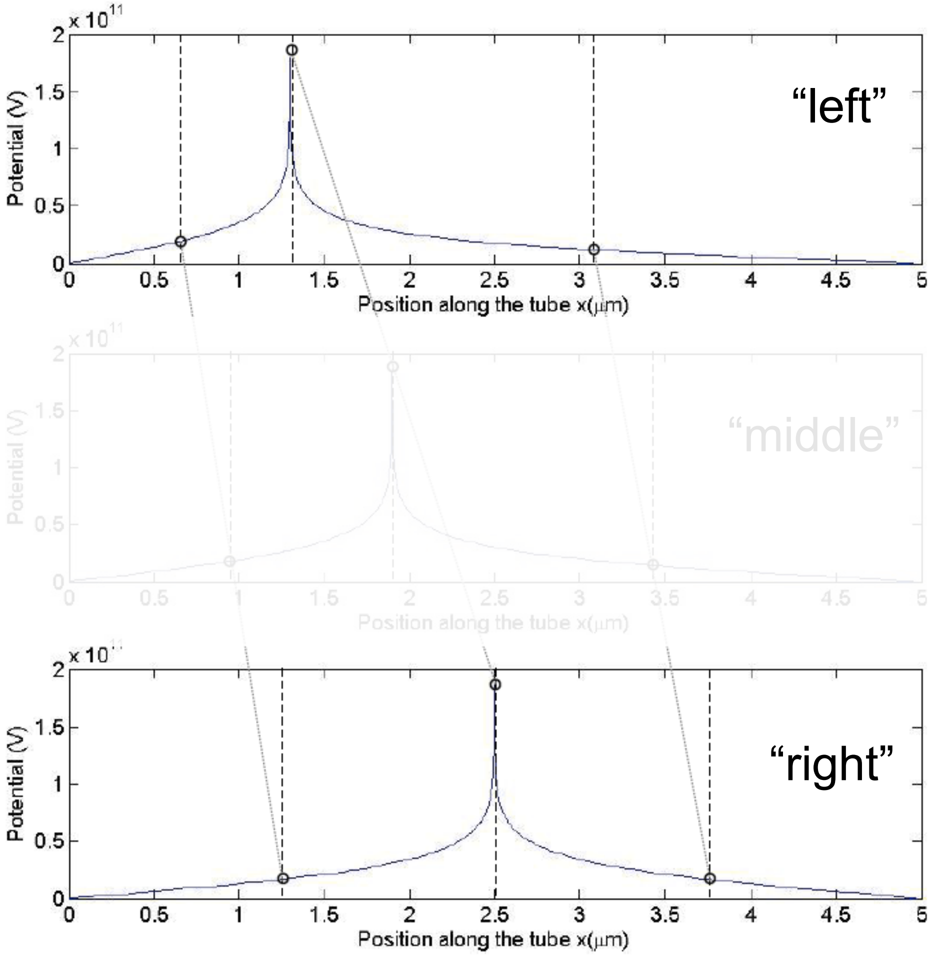
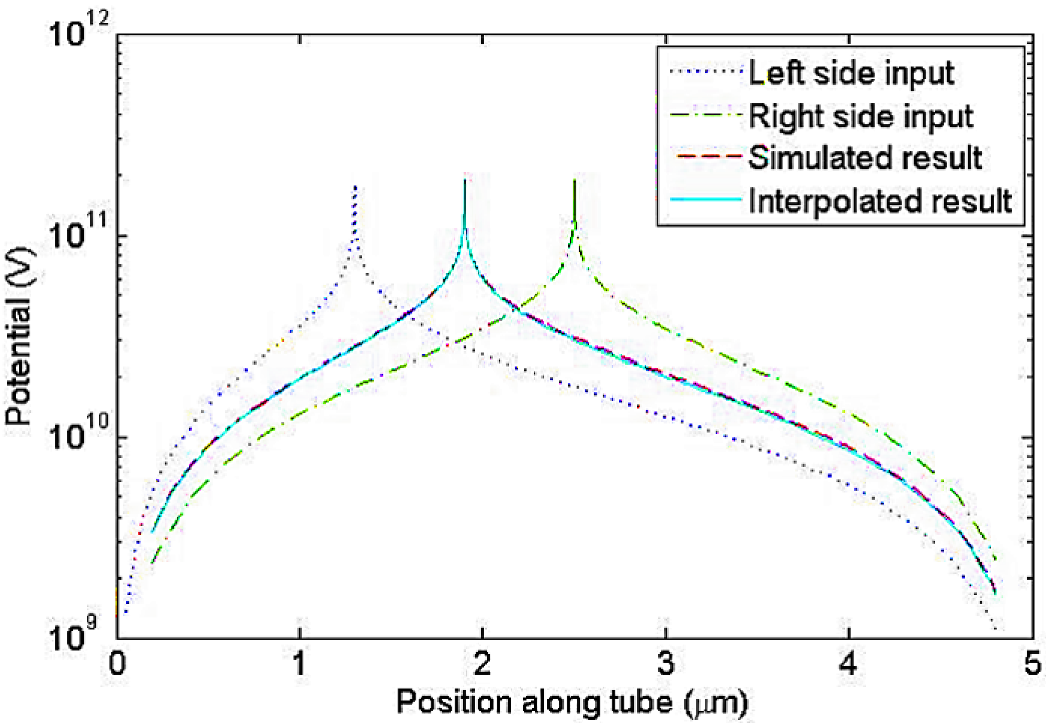
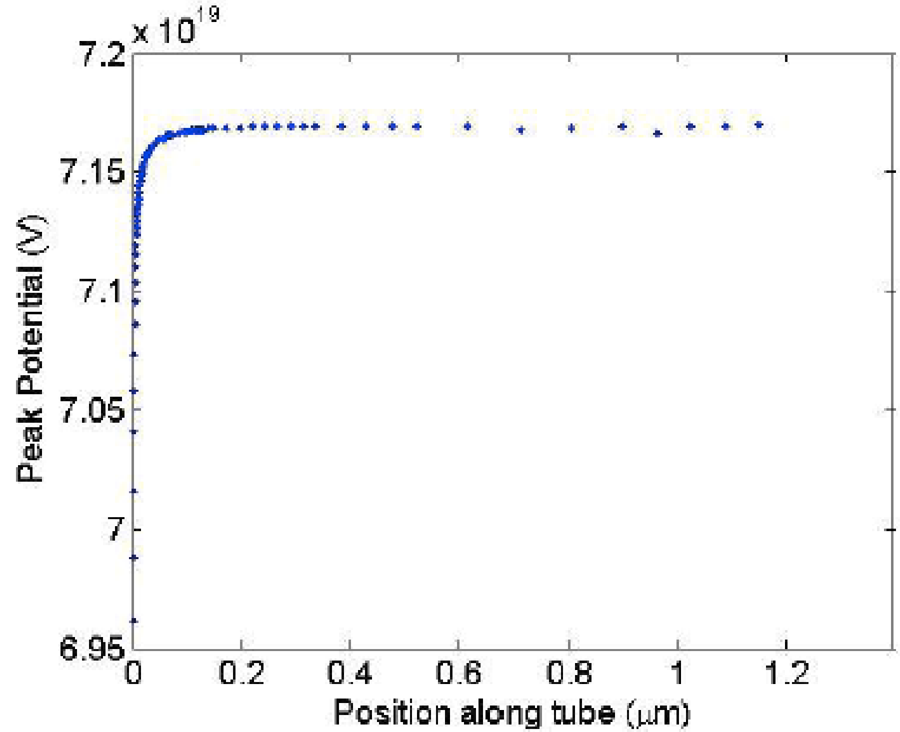
The “Warp” interpolation procedure



- Principle: if the potential due to “left” and “right” positions of the probe charge are known, the potential for a probe in the “middle” is obtained by shifting the “left”&”right” contours in the middle

The “Warp” interpolation results



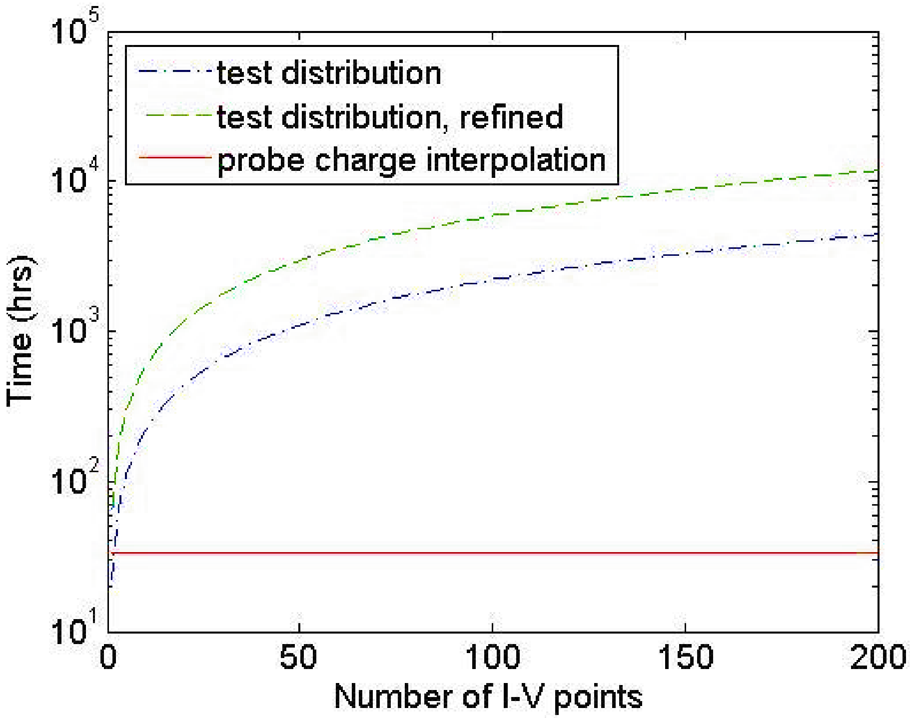


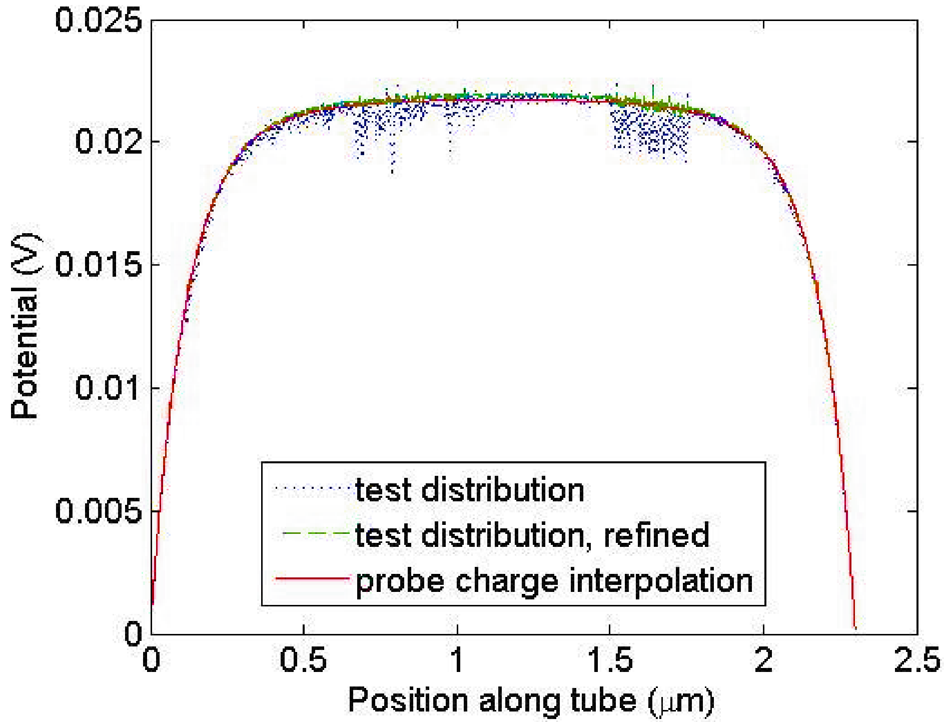
Within a 1% relative accuracy the “warp” interpolation reduces the number of probe charge positions (N) from ~7’500 to 97 (~80×)

Comparison of full 3D vs GF Poisson solver

$$q(x) = q_0 \exp\left(-\frac{|x - L/2|}{l_0}\right)\exp\left(-\frac{\sqrt{y^2 + z^2}}{\sigma^2}\right)$$

interpolation is 4s, full Poisson is 790s (2113s) and more accurate!





350× speed-up is possible in computing a 200 point I-V curve (assuming 100 self-consistent charge iterations)!

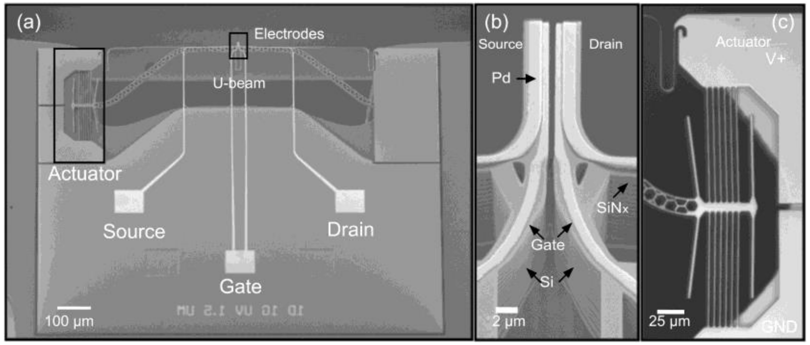
Conclusions and outlook

Conclusions

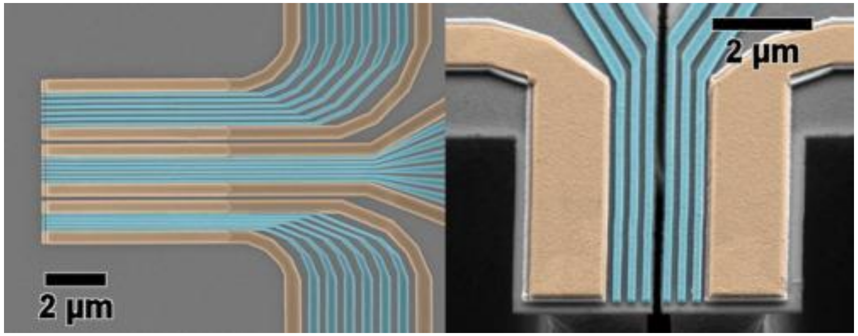
- Significant speed-up (350×) obtained in simulating 3D electrostatics by utilizing the Green's Function approach suggested here *(projected for 200 I-V point computation for 100 Poisson solutions per I-V point)*

Outlook

- Integrate the quantum transport solver to get I-V characteristics
- Model the mechanical/chemical aspects of the sensors
- Apply the modeling platform to various sensors based on carbon nanotubes



L. Kumar, Eurosensors 2017



L. Jenni *et al.*, Micr. Eng. 153, 105 (2016) [10.1016/j.mee.2016.03.013]

Thank you!

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