Undergraduate Research Project

Computer Modeling of Carbon-Nanotube Embedded Chemicapacitive Sensors

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Motivation

- For the past two and a half millennia **“the catapulting of plague victims to the deliberate use of infected clothes, insect vectors, and specialized weapon systems”** have been used to carry out offensive warfare.

- Shocking, real example: Anthrax attacks on the United States, 2002

- We aim to simulate a nanotube-embedded device able to detect small pathogenic particles with a high sensitivity and quick response rate.

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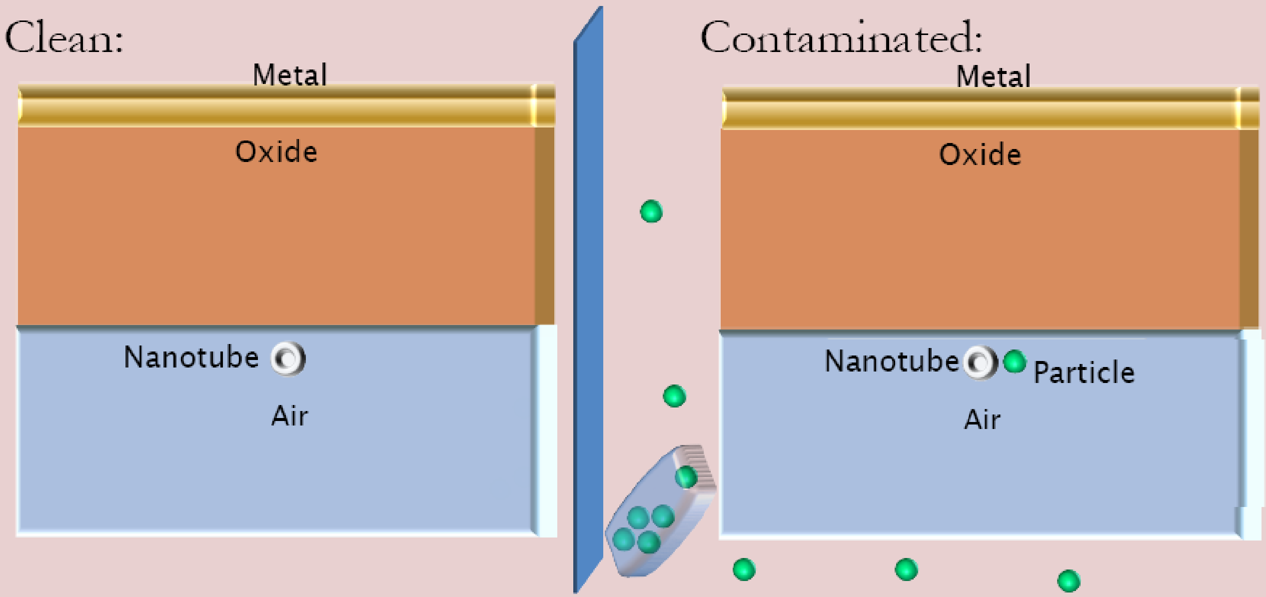
Sensor Design

Proposed Sensor Design



- Traditional capacitive sensor, was proposed by Delapierre in 1983.
- The sensitivity of the sensor is proportional to percent difference in capacitance before and after the particle enters.
- Proposed sensor replaces metal plate with a conducting carbon nanotube.

A Collaborative Effort

- Building a sensor is an involved, multi-faceted project:
  - Modeling of fundamental electrical properties
  - Chemical properties to ensure only the correct particles are detected
  - A probability analysis of the sensors' sucess
  - Prototypes; experimental and manufacturing design
- **Only the first goal was addressed in my work.**

- Work conducted under the direction of N. Goldsman and A. Akurk, University of Maryland, College Park.
- K. Dorsey (Olin College), M.S. Fuhrer (UMD), and A.E. Wickenden (ARL) contributed to the experimental study of this sensor.

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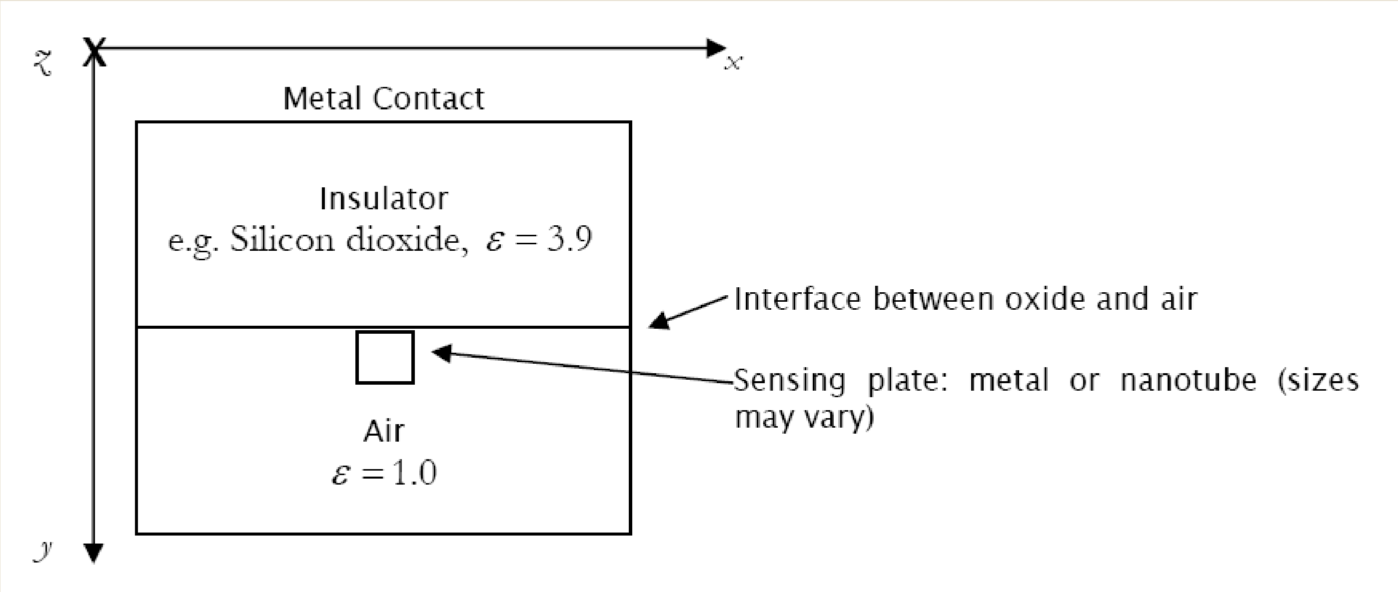
Numerical Model Overview



- We will numerically solve for potential using the Poisson equation in one, two, and three dimensions:

$\nabla \cdot (\varepsilon \nabla \phi) = -q\rho$ where

ϕ is the electrostatic potential; ε is the dielectric constant;

ρ is the net charge density; q is the electronic charge

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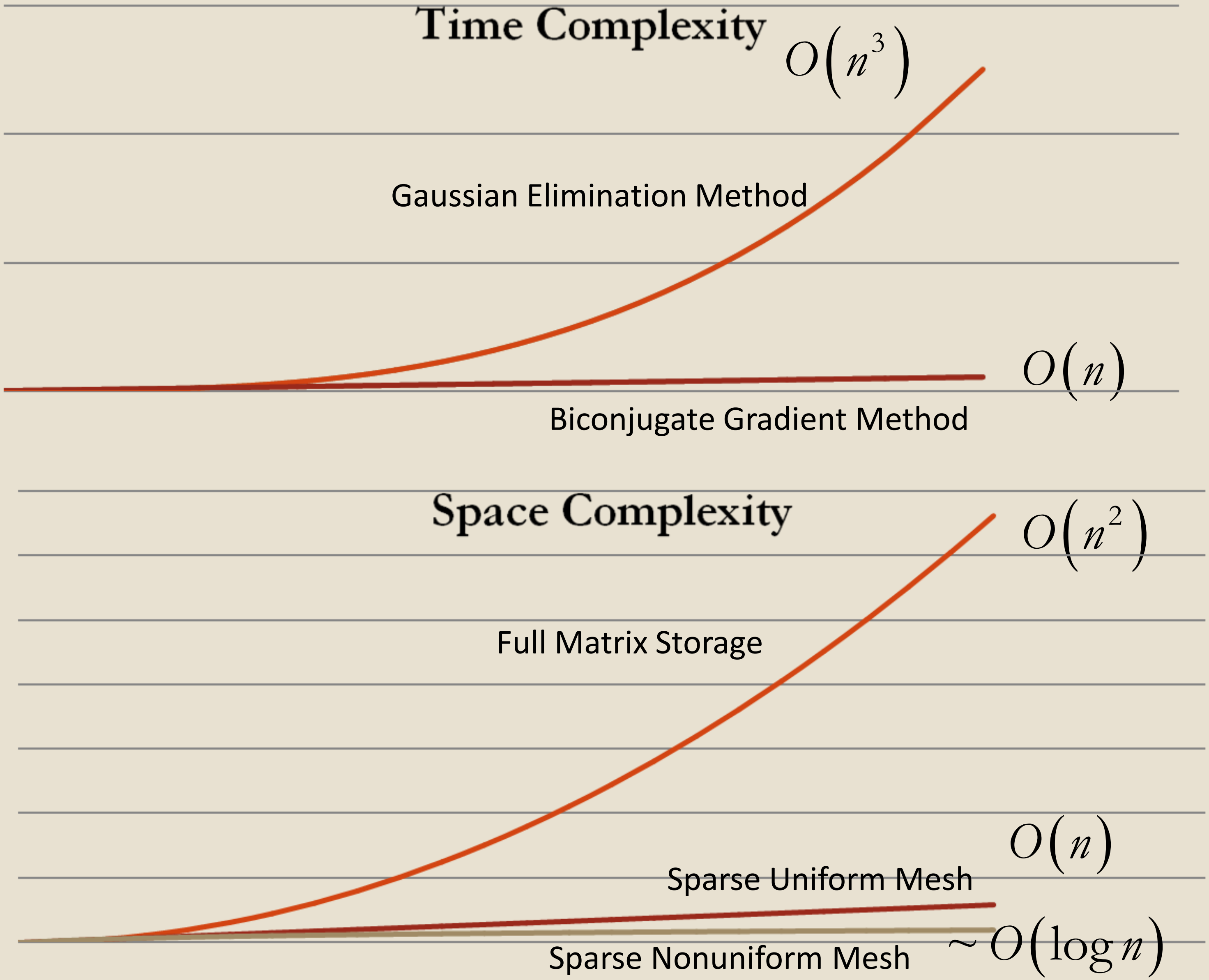
Computational Complexity for *n* Meshpoints



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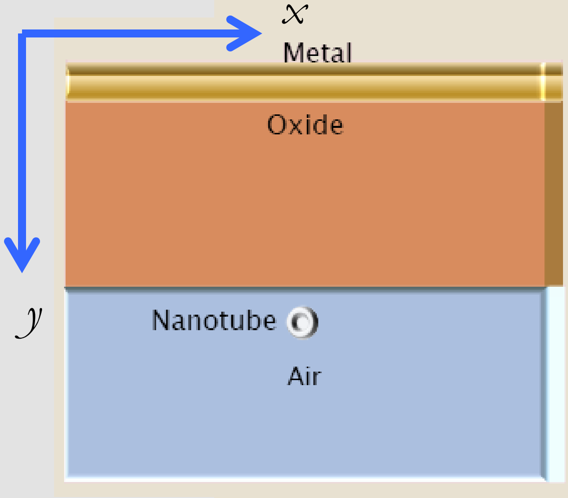
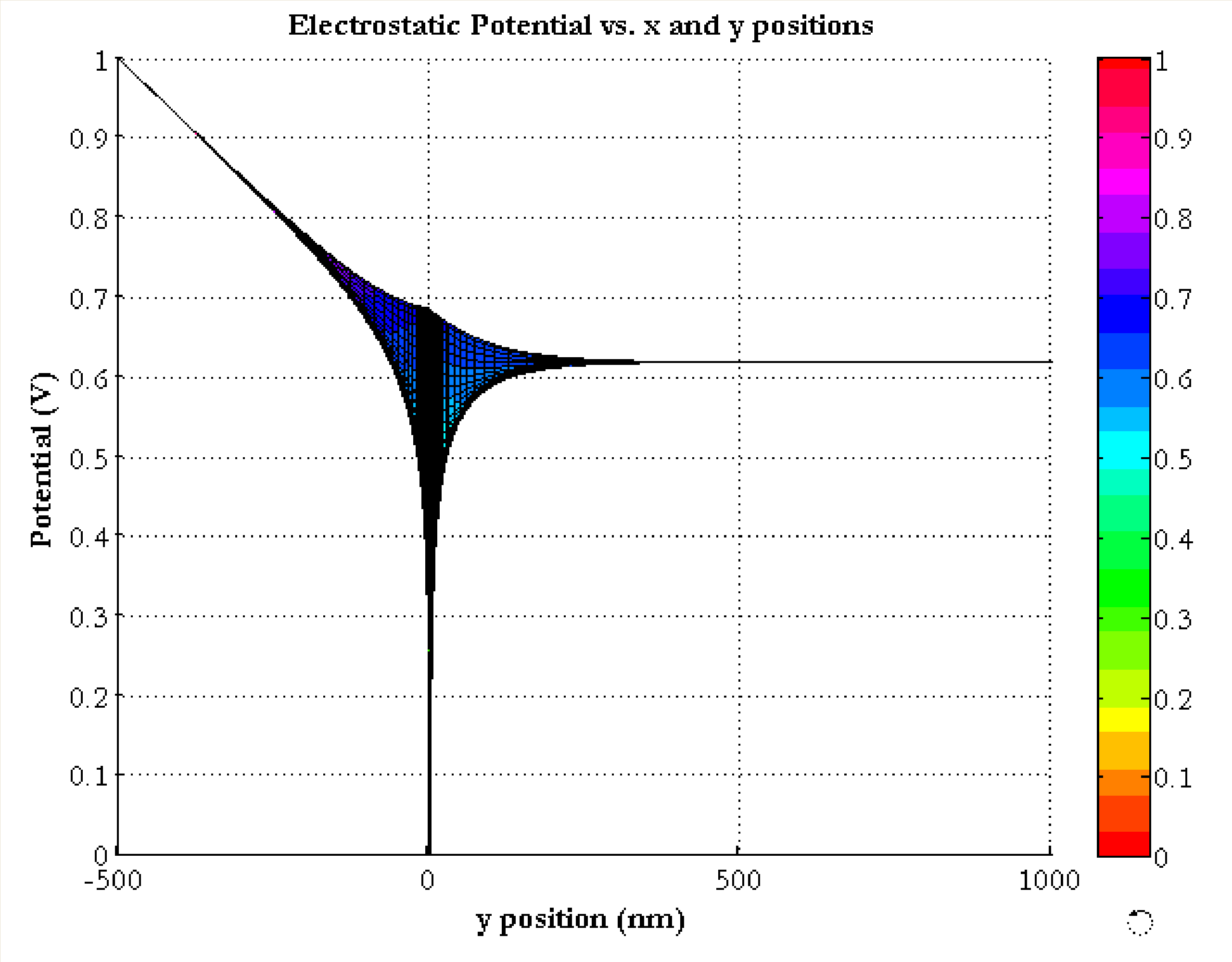
2D Case with Nanotube, Nonuniform Mesh





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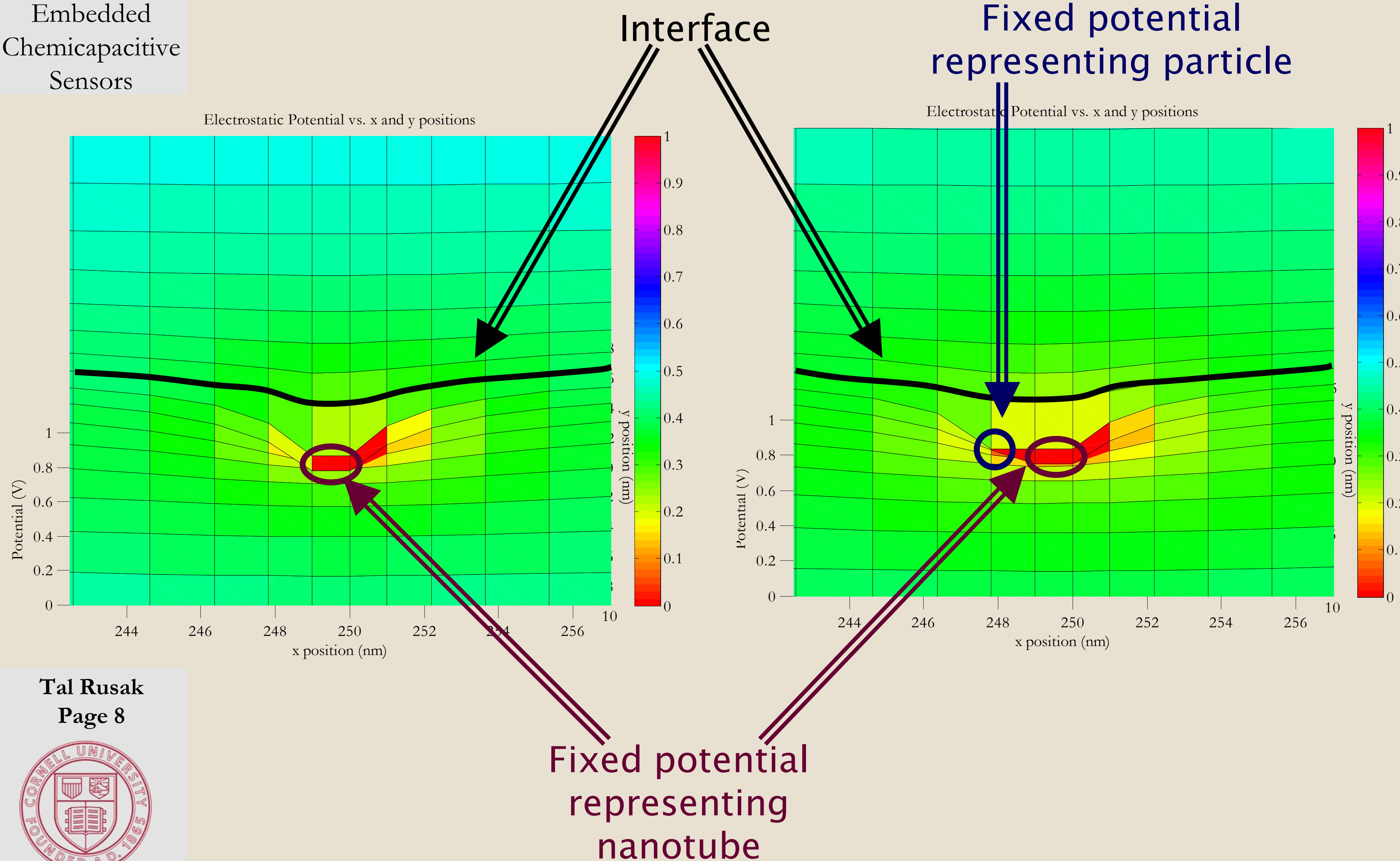
Nanotube and Particle Nonuniform Mesh



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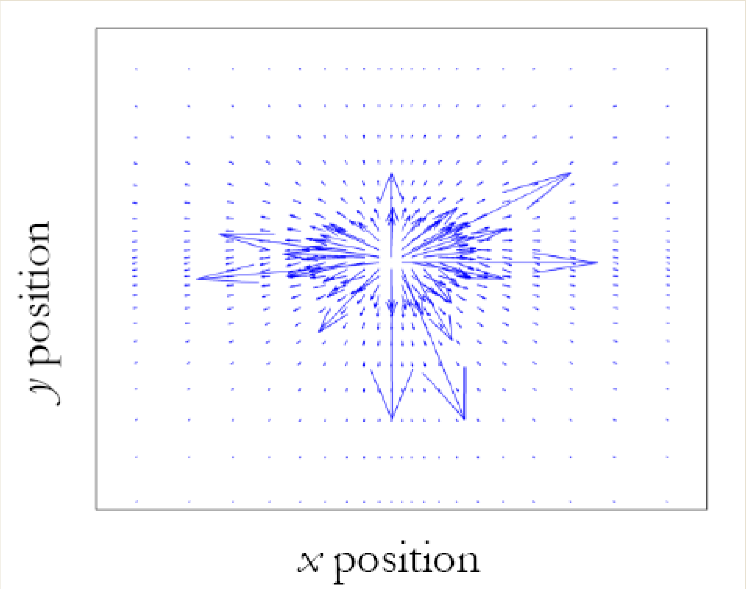
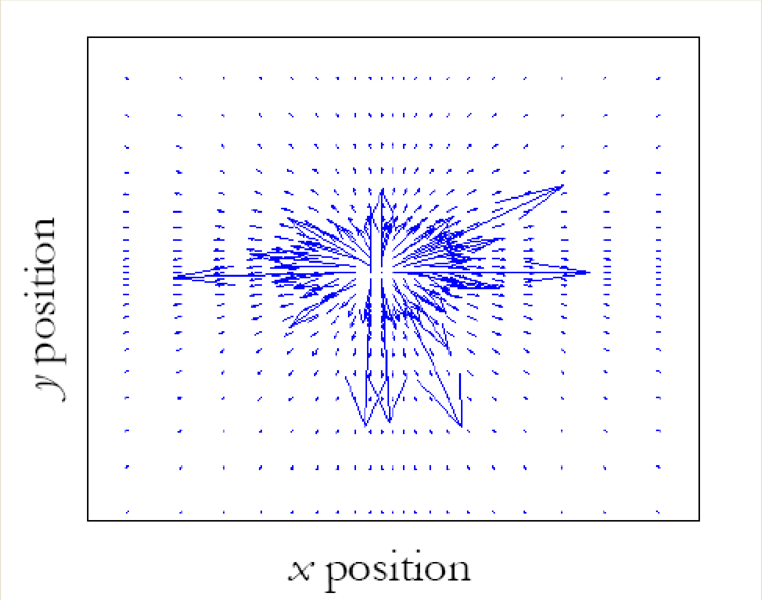
Electric Field and Capacitance

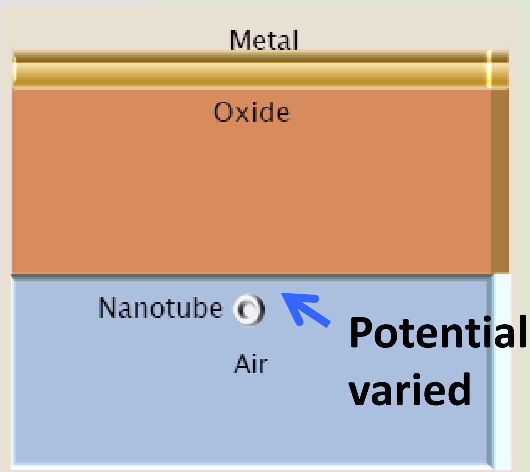
- Without particle:
  C = 0.127 pF/cm

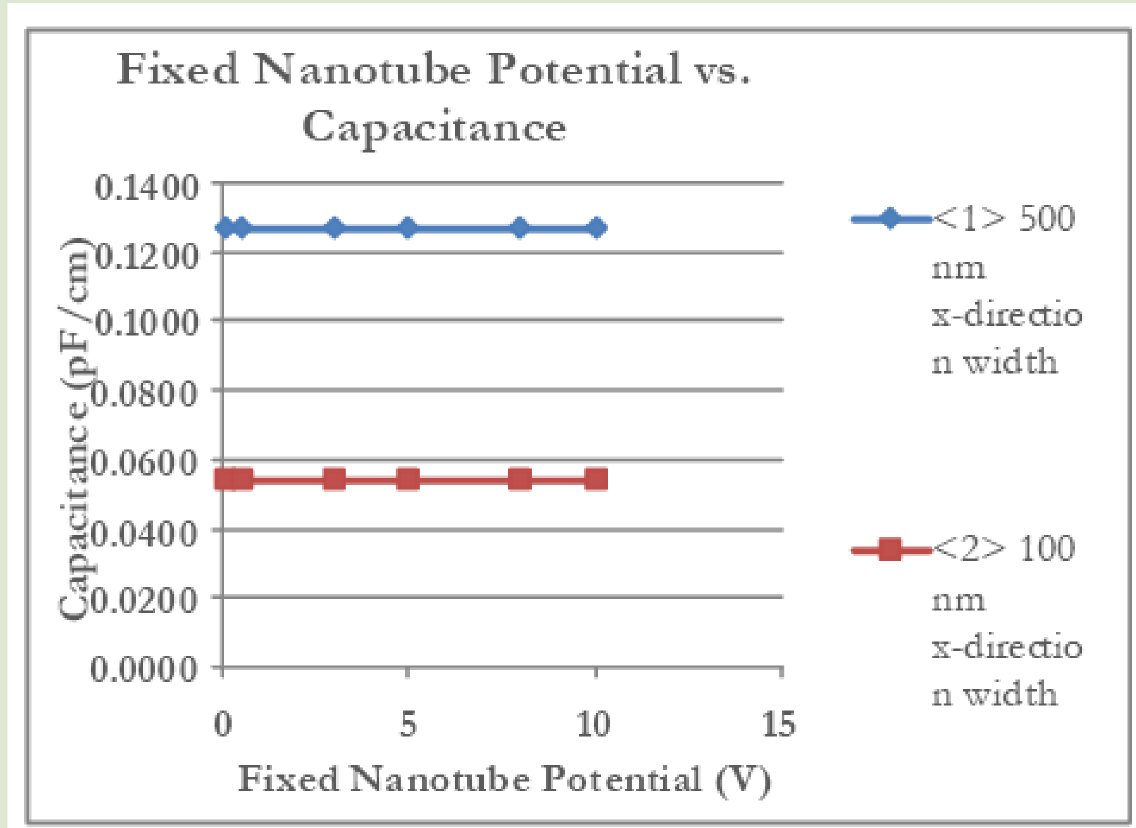


- With particle:
  C = 0.136 pF/cm



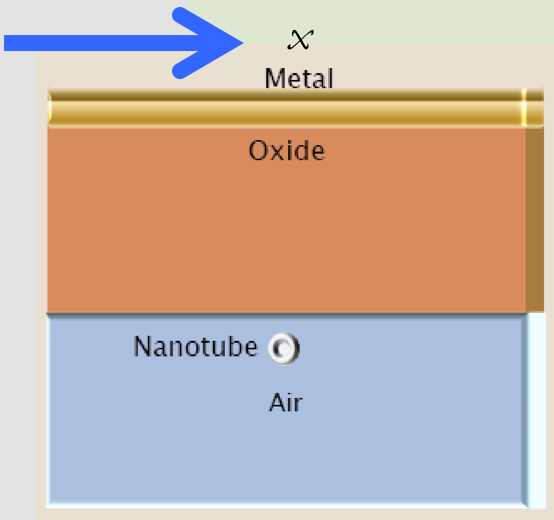
Effect of Nanotube Potential on Gate Capacitance

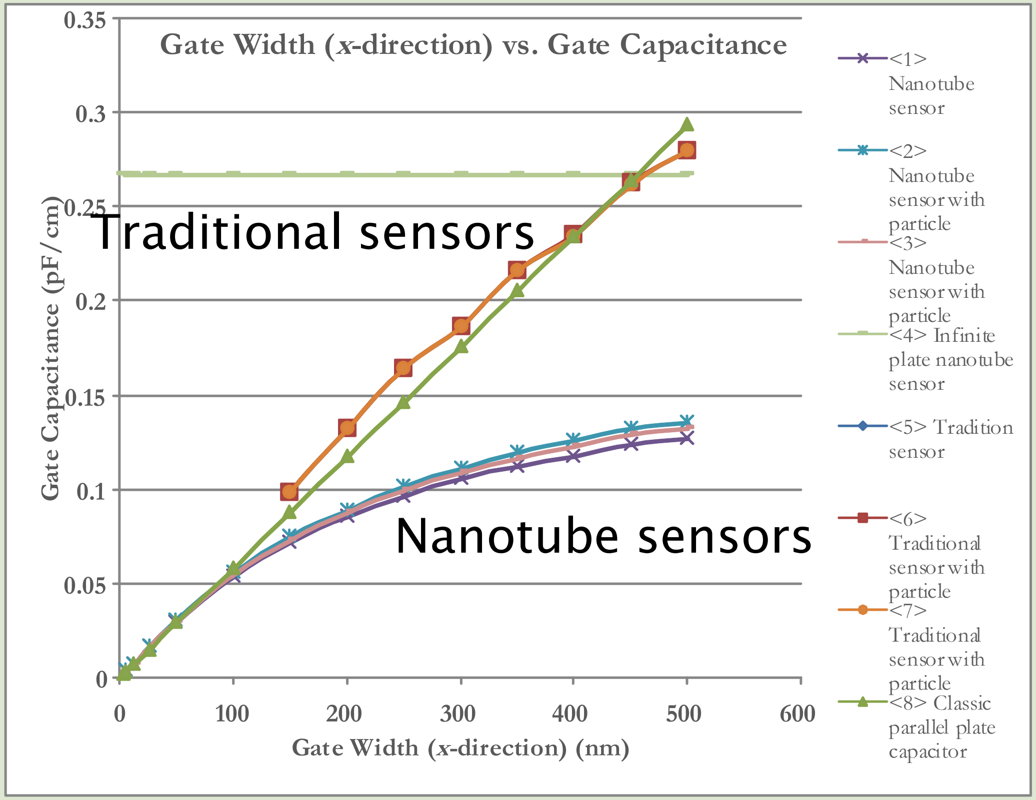




- The fixed potential of the nanotube has no impact on the gate capacitance.

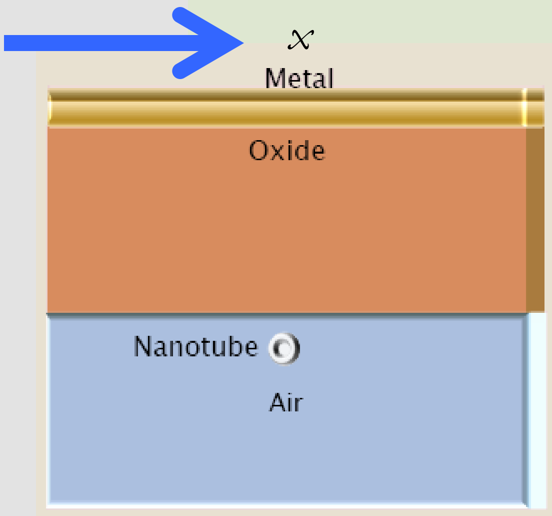
Effect of Gate Width (*x*-direction) on Capacitance

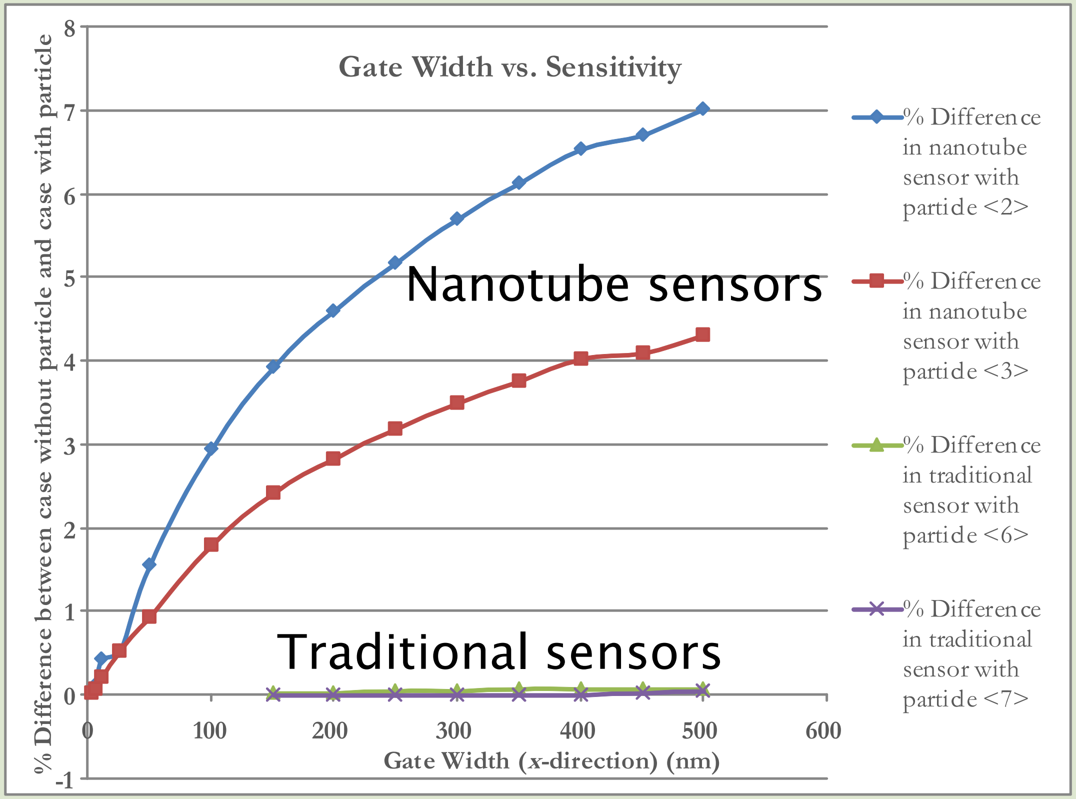




- Capacitance increases as gate width increases.
- The traditional sensor has a higher absolute capacitance.
- There is a greater *increase* in capacitance in the nanotube sensor.

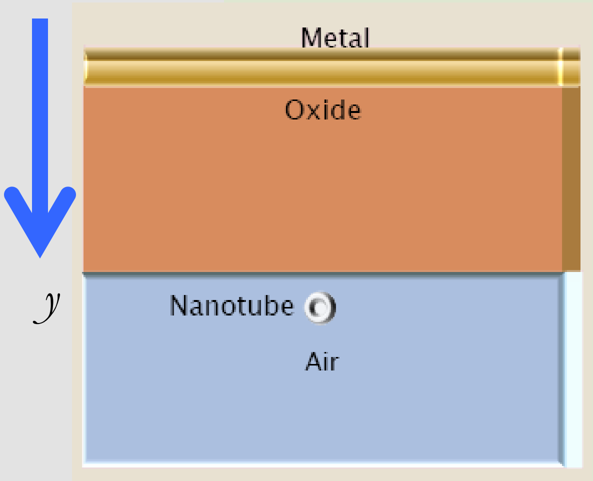
Effects of Gate Width (*x*-direction) on Sensitivity

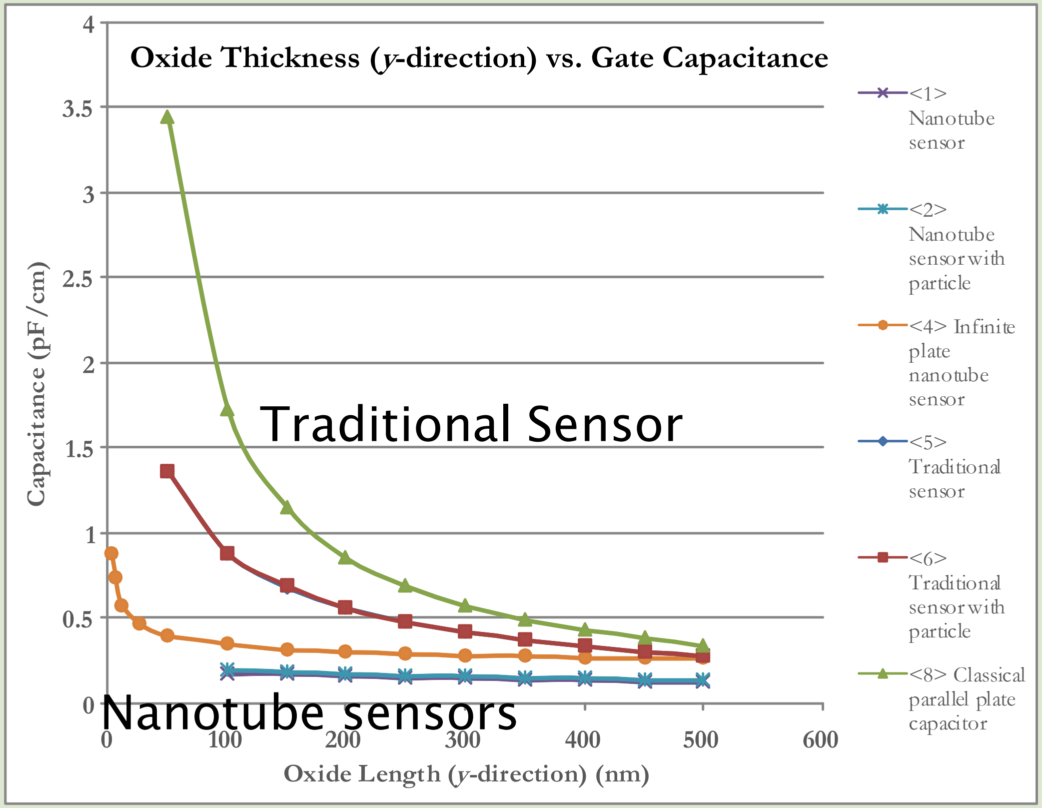




- The capacitance of nanotube sensors changes to a *much* greater extent than that of traditional sensors.
- Sensitivity increases as gate width (*x*-direction) increases.
- Sensitivity increases as distance to the interface decreases.

Effects of Oxide Thickness (*y*-direction) on Capacitance





- Gate capacitance decreases as oxide thickness increases.
- The traditional sensor has a higher absolute capacitance, but there is a larger *change* in capacitance in the nanotube sensor.

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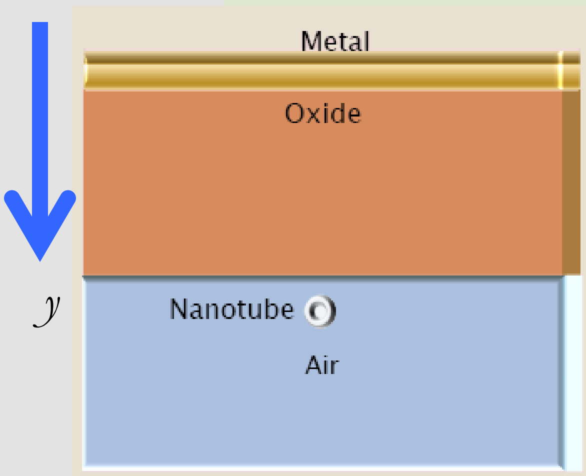
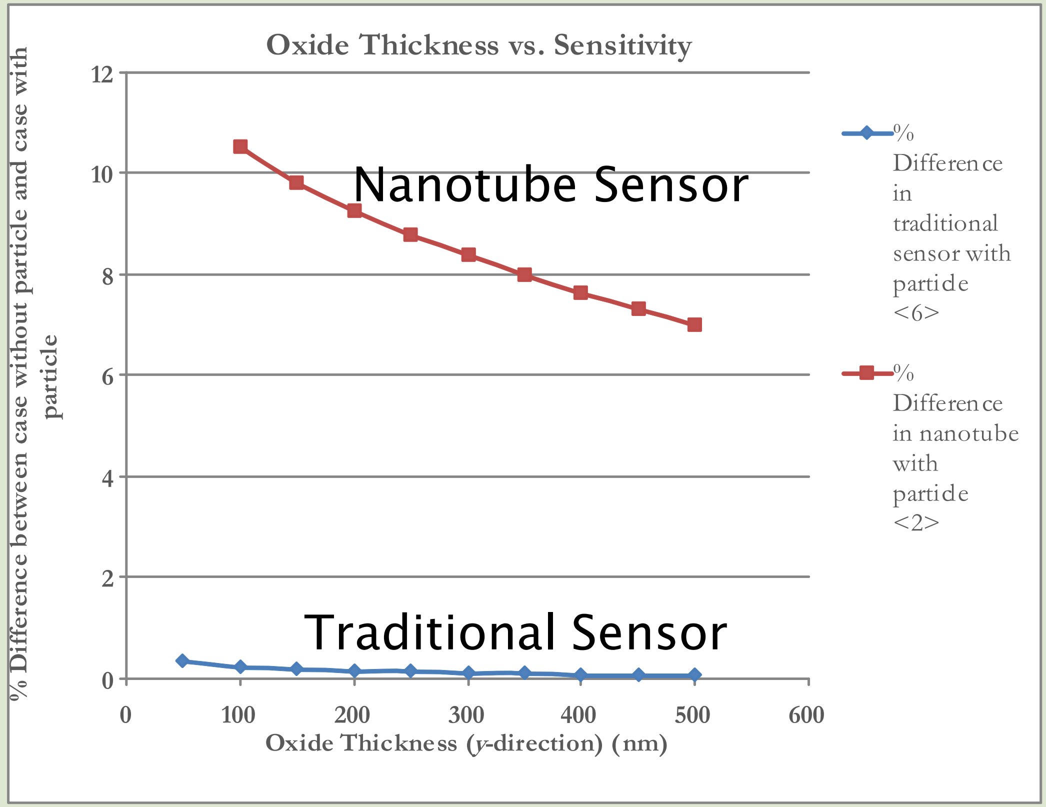
Effect of Oxide Thickness (*y*-direction) on Sensitivity





- As before, the nanotube sensor far exceeds the traditional sensor in terms of percent difference in capacitance.
- The percent difference decreases as oxide thickness (*y*-axis) increases.

Conclusions

- The numerical solutions show unequivocally that the proposed design for a nanotube sensor is advantageous over the traditional design in terms of percent difference upon the insertion of a particle, which leads to a higher sensitivity.

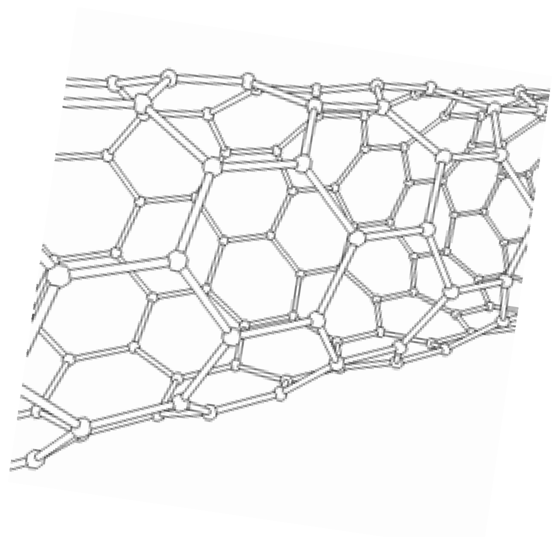
- The key advantages of such a development include the following:
  - Due to the small size of its components, the nanotube sensor will respond more quickly than a traditional sensor.
  - Detection of the desired particle will occur at a lower concentration and with far fewer particles.
  - Faster speed of detection will be experienced because the detector will be activated upon the entry of one particle, not many.

Thank you for your attention!

Questions?

Carbon Nanotubes (CNTs)

- The carbon nanotube was discovered by Sumio Iijima of NEC in 1991.
- A nanotube is a rolled sheet of graphene, which is in turn comprised of hexagonal rings of carbon atoms bonded in sp^2 hybridization.
- Advantageous in microelectronics because of a small size with a lower bound of 0.6 to 1.8 nm.
- We will study metallic CNTs in this work.



Schwarzm. (30 August 2004). Carbon nanotube. *August 1 2006,* Available: http://commons.wikimedia.org/wiki/Image:Kohlenstoffnanoroehre_Animation.gif. Used under GNU FDL

Meshes Used

- We use either a **uniform** or a **nonuniform** mesh to compute our linear approximation.
- In a **uniform mesh**, there is a constant spacing between points of a given direction.
- In a **nonuniform mesh**, the spacing between points is determined by the following equation

$$\begin{bmatrix} \cdots & \Delta p^3 & \Delta p^2 & \Delta p & \Delta & \Delta & \Delta p & \Delta p^2 & \Delta p^3 & \cdots \end{bmatrix}$$

where p and Δ are constants in a given direction.

In all examples given in this presentation, $p_x = p_y = 1.2$ and $\Delta_x = \Delta_y = 1.0$.

Equations for Uniform Mesh Solutions

- One dimensional uniform mesh

$$\varepsilon(y-\Delta/2)\phi(y-\Delta)-\left(\varepsilon(y+\Delta/2)+\varepsilon(y-\Delta/2)\right)\phi(y) + \varepsilon(y+\Delta/2)\phi(y+\Delta)=0$$

- Two dimensional uniform mesh

$$\varepsilon\begin{pmatrix} x \\ y-\Delta/2 \end{pmatrix}\phi\begin{pmatrix} x \\ y-\Delta \end{pmatrix}+\varepsilon\begin{pmatrix} x-\Delta/2 \\ y \end{pmatrix}\phi\begin{pmatrix} x-\Delta \\ y \end{pmatrix}$$

$$-\left(\varepsilon\begin{pmatrix} x \\ y+\Delta/2 \end{pmatrix}+\varepsilon\begin{pmatrix} x+\Delta/2 \\ y \end{pmatrix}+\varepsilon\begin{pmatrix} x \\ y-\Delta/2 \end{pmatrix}+\varepsilon\begin{pmatrix} x-\Delta/2 \\ y \end{pmatrix}\right)\phi\begin{pmatrix} x \\ y \end{pmatrix}$$

$$+\ \varepsilon\begin{pmatrix} x+\Delta/2 \\ y \end{pmatrix}\phi\begin{pmatrix} x+\Delta \\ y \end{pmatrix}+\varepsilon\begin{pmatrix} x \\ y+\Delta/2 \end{pmatrix}\phi\begin{pmatrix} x \\ y+\Delta \end{pmatrix}=0$$

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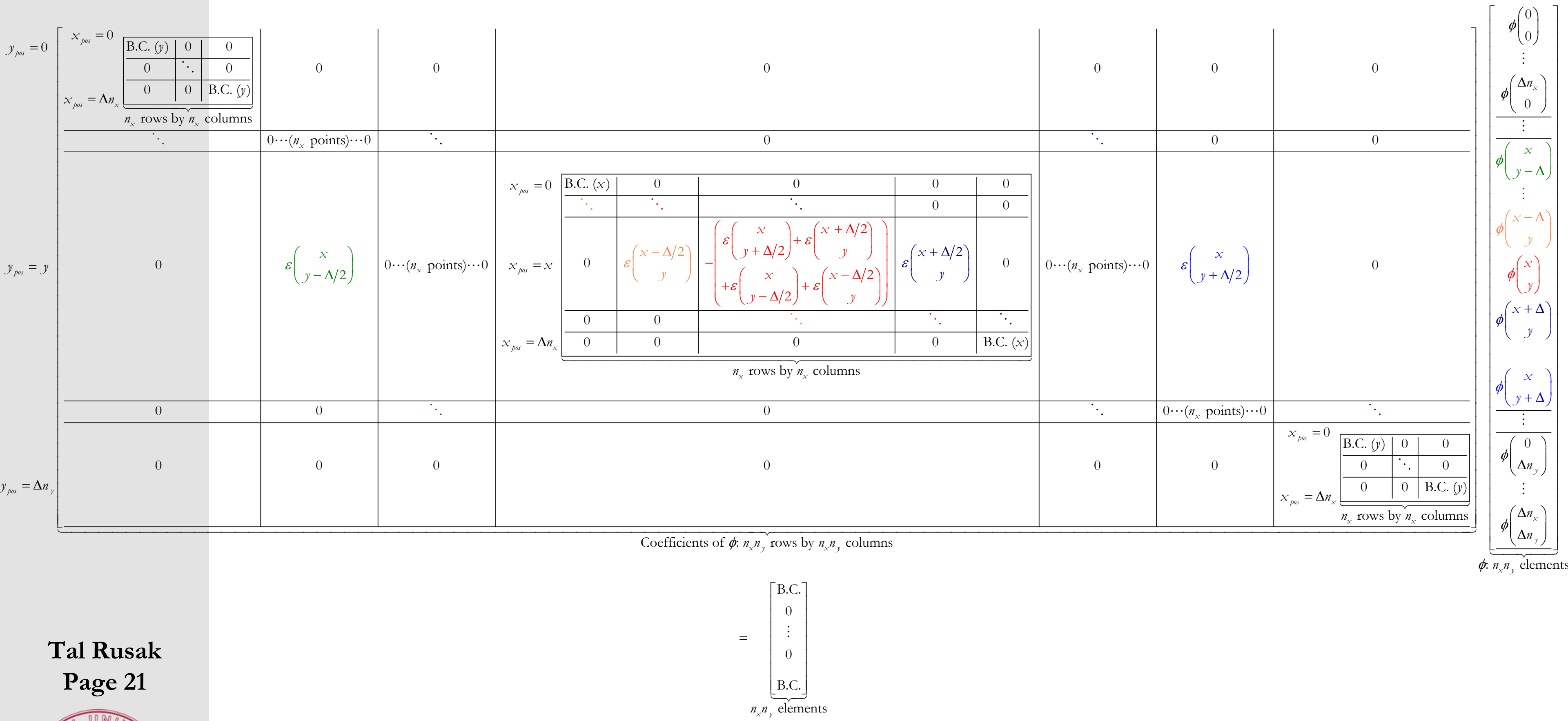
Matrix for 1D Uniform Solution

$$
\begin{array}{r}
y_{pos}=0 \\ \\ \\ \vdots \\ \\ \\ y_{pos}=\Delta n_y
\end{array}
\underbrace{\begin{bmatrix}
\text{Boundary condition} & 0 & 0 & 0 & 0 & 0 & 0 \\
\ddots & \ddots & \ddots & 0 & 0 & 0 & 0 \\
0 & \ddots & \ddots & \ddots & 0 & 0 & 0 \\
0 & 0 & \varepsilon(y-\Delta/2) & -\begin{pmatrix}\varepsilon(y+\Delta/2) \\ +\varepsilon(y-\Delta/2)\end{pmatrix} & \varepsilon(y+\Delta/2) & 0 & 0 \\
0 & 0 & 0 & \ddots & \ddots & \ddots & 0 \\
0 & 0 & 0 & 0 & \ddots & \ddots & \ddots \\
0 & 0 & 0 & 0 & 0 & 0 & \text{Boundary condition}
\end{bmatrix}}_{\text{Coefficients of } \phi\text{: } n_y \text{ rows by } n_y \text{ columns}}
\underbrace{\begin{bmatrix}
\phi(0) \\ \vdots \\ \phi(y-\Delta) \\ \phi(y) \\ \phi(y+\Delta) \\ \vdots \\ \phi(\Delta n_y)
\end{bmatrix}}_{\phi\text{: } n_y \text{ elements}}
=
\underbrace{\begin{bmatrix}
\text{Boundary condition} \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ \text{Boundary condition}
\end{bmatrix}}_{n_y \text{ elements}}
$$

Matrix Used for 2D Uniform Solution



Equations for Nonuniform Mesh Solutions

- Interface Equation (all nonuniform meshes):

$$\frac{\varepsilon_{oxide}}{\Delta_y(j-1)}\phi\left(y_0-\Delta_y(j)\right)-\left(\frac{\varepsilon_{oxide}}{\Delta_y(j-1)}+\frac{\varepsilon_{air}}{\Delta_y(j)}\right)\phi\left(y_0\right)$$

$$+\frac{\varepsilon_{air}}{\Delta_y(j)}\phi\left(y_0+\Delta_y(j)\right)=0$$

- Two dimensional nonuniform mesh

$$\frac{2}{\Delta_y(j-1)\left(\Delta_y(j)+\Delta_y(j-1)\right)}\phi\begin{pmatrix}x\\ y-\Delta_y(j)\end{pmatrix}+\frac{2}{\Delta_x(i-1)\left(\Delta_x(i)+\Delta_x(i-1)\right)}\phi\begin{pmatrix}x-\Delta_x(i)\\ y\end{pmatrix}$$

$$-\left(\frac{2}{\Delta_x(i-1)\Delta_x(i)}+\frac{2}{\Delta_y(j-1)\Delta_y(j)}\right)\phi\begin{pmatrix}x\\ y\end{pmatrix}+\frac{2}{\Delta_x(i)\left(\Delta_x(i)+\Delta_x(i-1)\right)}\phi\begin{pmatrix}x+\Delta_x(i)\\ y\end{pmatrix}$$

$$+\frac{2}{\Delta_y(j)\left(\Delta_y(j)+\Delta_y(j-1)\right)}\phi\begin{pmatrix}x\\ y+\Delta_y(j)\end{pmatrix}=0$$

Equations for Nonuniform Mesh Solutions

- Three dimensional nonuniform mesh

$$
\begin{aligned}
&\frac{2}{\Delta_y(j-1)\left(\Delta_y(j)+\Delta_y(j-1)\right)}\phi\begin{pmatrix} x \\ y-\Delta_y(j) \\ z \end{pmatrix} + \frac{2}{\Delta_x(i-1)\left(\Delta_x(i)+\Delta_x(i-1)\right)}\phi\begin{pmatrix} x-\Delta_x(i) \\ y \\ z \end{pmatrix} \\
&+\frac{2}{\Delta_z(k-1)\left(\Delta_z(k)+\Delta_z(k-1)\right)}\phi\begin{pmatrix} x \\ y \\ z-\Delta_z(k) \end{pmatrix} \\
&-\left(\frac{2}{\Delta_x(i-1)\Delta_x(i)}+\frac{2}{\Delta_y(j-1)\Delta_y(j)}+\frac{2}{\Delta_z(k-1)\Delta_z(k)}\right)\phi\begin{pmatrix} x \\ y \\ z \end{pmatrix} \\
&+\frac{2}{\Delta_x(i)\left(\Delta_x(i)+\Delta_x(i-1)\right)}\phi\begin{pmatrix} x+\Delta_x(i) \\ y \\ z \end{pmatrix} + \frac{2}{\Delta_y(j)\left(\Delta_y(j)+\Delta_y(j-1)\right)}\phi\begin{pmatrix} x \\ y+\Delta_y(j) \\ z \end{pmatrix} \\
&+\frac{2}{\Delta_z(k)\left(\Delta_z(k)+\Delta_z(k-1)\right)}\phi\begin{pmatrix} x \\ y \\ z+\Delta_z(k) \end{pmatrix} = 0
\end{aligned}
$$

Boundary Conditions

- We will use both Dirichlet and Neumann boundary conditions in this work.
- In a **Dirichlet (fixed)** boundary, potential is set to a constant, i.e.,
  $\phi = c.$
- In a **Neumann (floating)** boundary, the *derivative* of the potential is constant in a direction perpendicular to the boundary, e.g., if the bottom x boundary of the MOS is floating, then its boundary condition will be $\partial\phi/\partial y = 0$, since the y-axis is perpendicular to the x-axis.

Methods of Computing the Solution

- n is defined as $n = n_x n_y$ in 2D and $n = n_x n_y n_z$ in 3D
- We can solve for potential using the **Gauss-Jordan Elimination** method. The implementation used requires the storage of all elements of the matrix and vectors required to solve the equation.
  - Time complexity: $O(n^3)$
  - Space complexity: $(8 \text{ bytes})(n^2 + 2n) = O(n^2)$
- To save time and space, we used indexed storage along with the **biconjugate gradient** method. Only elements in the main diagonal and the nonzero offdiagonal elements of the matrix are stored. Time complexity: $O(n)$
  - Space complexity: In 2D case:

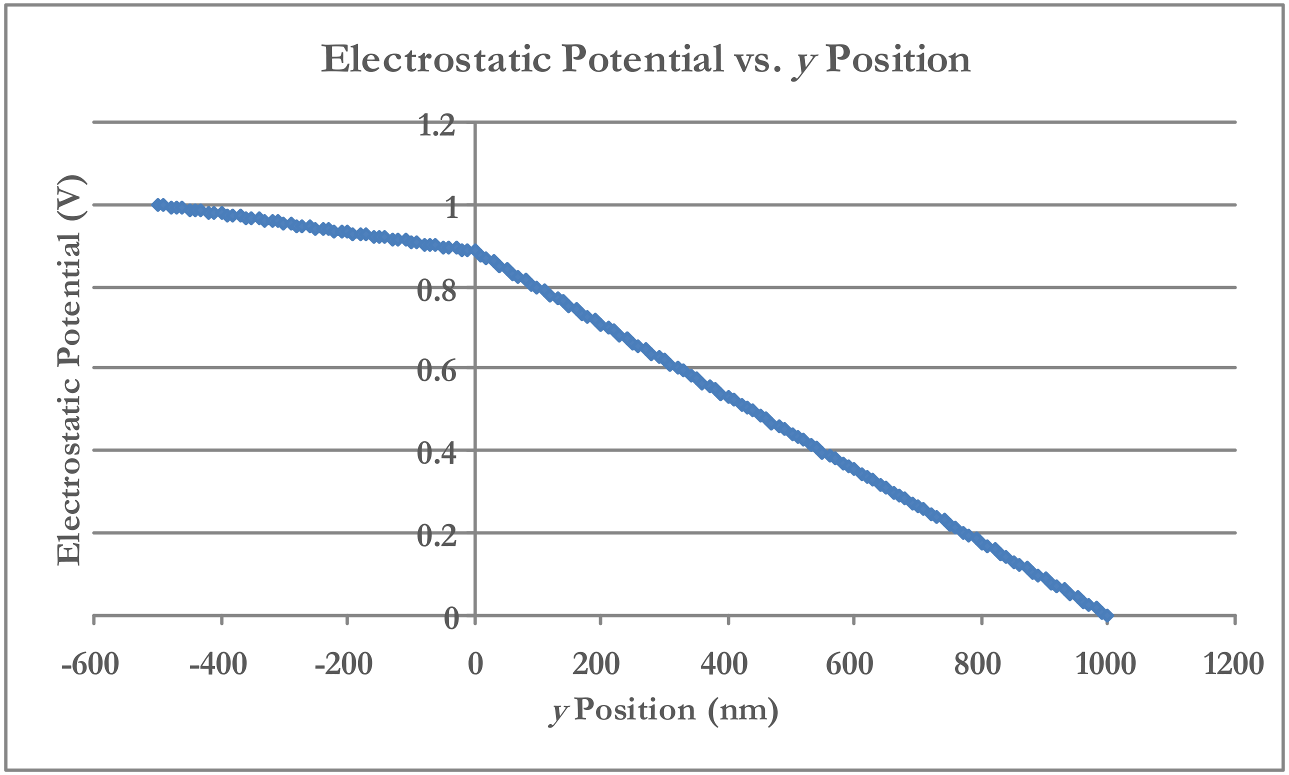
    $$5n(8 \text{ bytes}) + 5n(4 \text{ bytes}) + n(8 \text{ bytes}) + n(8 \text{ bytes}) = O(n)$$

    In 3D case:

    $$7n(8 \text{ bytes}) + 7n(4 \text{ bytes}) + n(8 \text{ bytes}) + n(8 \text{ bytes}) = O(n)$$

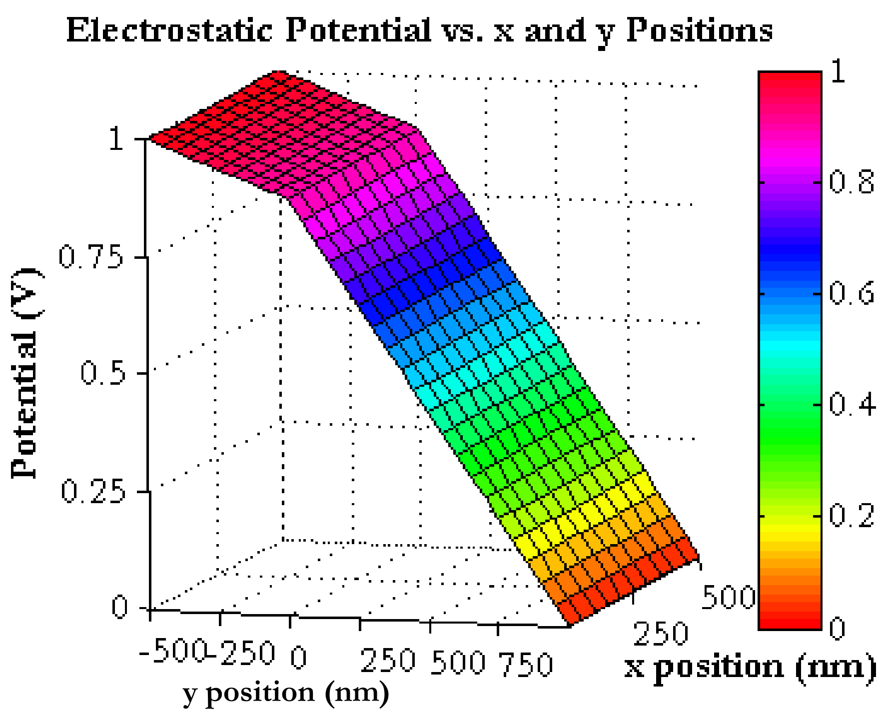
One Dimensional Case Uniform Mesh

- **Problem statement:** We choose a device that has a 500 nm oxide ($\varepsilon = 4.5$) and 1000 nm of air ($\varepsilon = 1.0$). We use fixed boundary conditions: the left potential is set to 1 V; the right is set to 0 V. $n_y = 151$



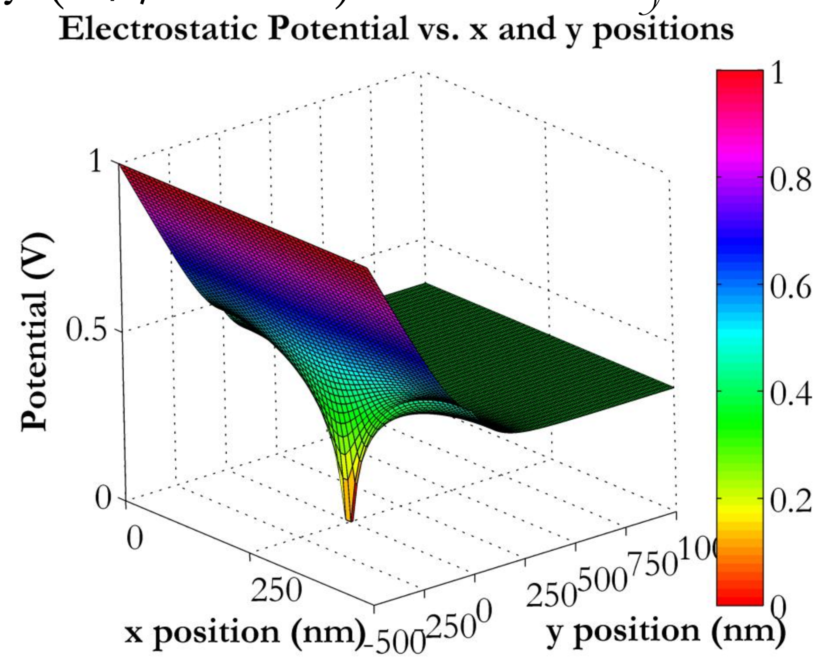
Two Dimensional Case Uniform Mesh

- The device is partitioned along the y direction, 500 nm for silicon dioxide ($\varepsilon = 3.9$) and 1000 nm for air ($\varepsilon = 1.0$). The device width in the x direction is 500 nm and there is no nanotube or sensing plate. Our boundary conditions are fixed on the y boundaries (1 V at $y = -500$ nm and 0 V at $y = 1000$ nm) and are floating on the x boundaries $\left(\partial\phi/\partial y = 0\right)$. $n_y = 31$, $n_x = 11$



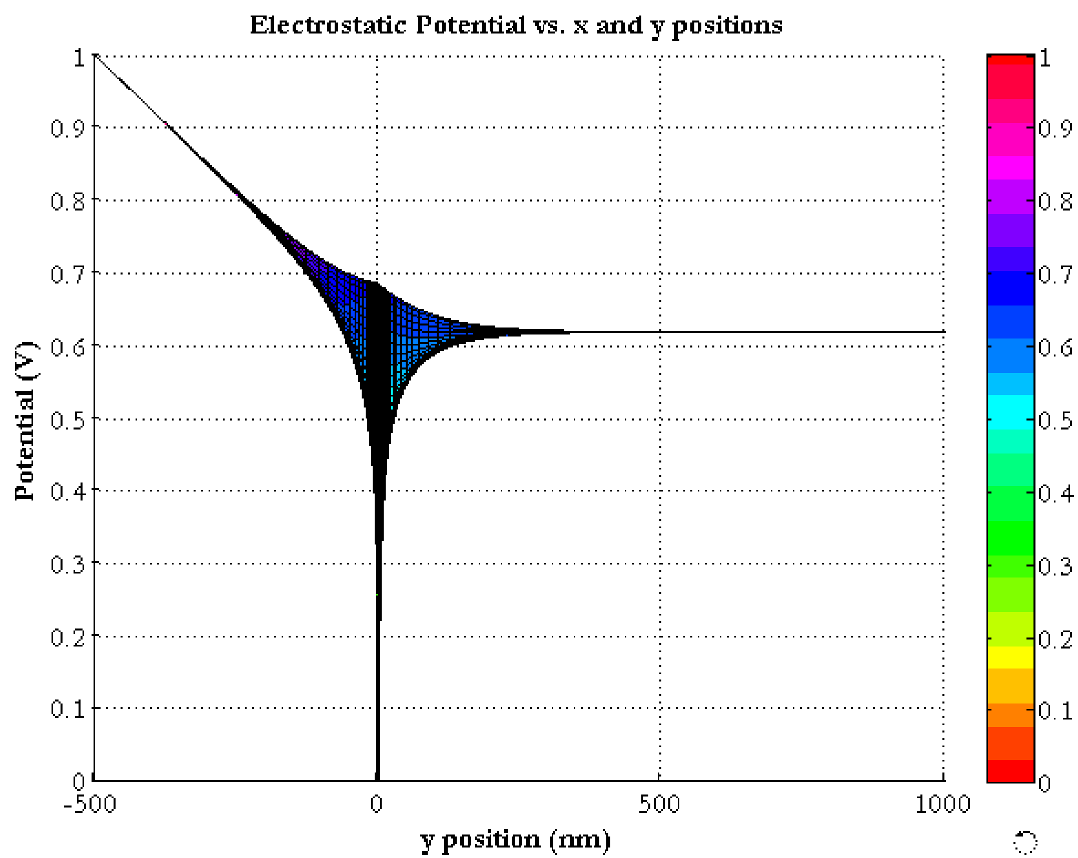
2D Case with Nanotube Uniform Mesh

- **Problem statement:** We now introduce a nanotube. This nanotube will be represented by four meshpoints (20 nm by 20 nm square) of a fixed potential (0 V) at a distance of 1 nm from the interface of the oxide and air, inside the air. The physical dimensions of the figure are the same as in the previous problem, as are all boundary conditions except the bottom boundary in the *y* direction, which is changed to a floating boundary $\left(\partial\phi/\partial x = 0\right)$. $n_y = 151, n_x = 51$
- Capacitance = 0.215 pF/cm



2D Case with Nanotube Nonuniform Mesh

- **Problem statement:** Same problem as before, but the nonuniform mesh enables us to insert a 2 nm by 2 nm nanotube, which is more realistic in size.



- Capacitance = 0.127 pF/cm

Three Dimensional Solution Nonuniform Mesh

- The two dimensional problem solved (without particle) is extended to 3D. The z boundary conditions are floating around CNT and fixed elsewhere.