1. **The prior knowledge of the students willing to attend the tutorial**

Elasticity theory: Young's modulus, stress tensor etc. Mechanical oscillations, eigenfrequencies.

2. **The tools necessary to participate in the tutorial (computer, writing utensils, specific software, etc…**

Computer, COMSOL Multiphysics software

3. **The content of the tutorial planned over the length of the requested tutorial time slot (tentative divisions, how much time you want to devote to each part)**

* Setting up COMSOL for mechanical simulations
(done beforehand preferrably, but takes about 1 min.)
1) Simulating a Si nanobeam: ***(10 minutes)***
* Selecting the right kind of simulation (Eigenfrequency)
* Building the geometry
* Selecting the material
* Defining the boundary conditions (both ends of the beam are fixed)
* Building the mesh
* Running the simulation & computing eigenfrequencies
(up to 5 minutes dedicated to everything until this part)
* Comparing the simulated eigenfrequencies with analytical results
(up to 5 minutes dedicated to this last part)
2) Simulating a SiN string under strain: ***(as much as can be fit in 10 minutes)***
* Selecting the right kind of simulation (Stationary)
* Building the geometry
* Selecting the material
* Defining the boundary conditions
* Building the mesh
* Running the simulation & computing the displacement
(I expect the part until now to take 5 minutes)
* Changing the colour scale
* Building a 1D plot of the displacement
* Adding initial stress of SiN to the simulation
* Rerunning the simulation
* Building a 2D plot of the stress
* Calculating the average stress in one direction

The detailed plan is as follows:

Introduction to COMSOL - Modelling Nanostructures

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Based on Nano- and Optomechanics course by Prof. Dr. Menno Poot (Technical University of Munich)

Finding the eigenmodes of a silicon beam

Remember to save your work regularly!

1. The first step is to select the right kind of simulation.
 a. Select, ModelWizard, 3D, expand Structural Mechanics, select Solid Mechanics, click Add
 b. As shown, this will calculate the displacement field (u,v,w)
 c. Click Study
 d. Select Eigenfrequency, Done

2. Now you see the main window of COMSOL. The top menu contains the thematically grouped items that you can select. Typically, you work through them left to right. When adding something, it appears in the panel on the left side. Note that the same names appear here, as in the menu. For clarity, I will indicate things that you do in the menu as normal text and actions in the ”Model builder” panel in *italics*.

3. Next we will build the geometry
a. Name the geometry e.g. fiSilicon nanobeamfl (this step is not very important but helps in more complicated geometries)
b. Select the Geometry menu
c. Select Block
d. A new panel appears where you can set the properties of the Block.
e. Label it “Beam”, and set w = 10 um, d = 500 nm, h = 200 nm (the width correspond to the x direction). You can use either the notation 500e-9 or 500 [nm] to indicate dimensions, e.g. the “depth” of the beam (y direction).
f. Change position → base to Center
g. Click Build all objects. The beam now appears in the blueish panel. You can rotate it around with the mouse, and zoom in and out using the first five icons.
Hint: If you messed up the orientation or zoom, simply click on the 6th icon with the three colored axes to get the default view back.

4. Now we have to select the material. This is the next menu item (remember how we always go from left to right in the COMSOL workflow).
a. Click blank material (with add material you can search in a database with predefined materials)
b. In the second panel, we can now enter the desired material properties. Label it “our silicon”. Go to “Material contents” and set E=130 GPa, nu = 0.28, rho = 2330 kg/m^3.*
c. Select the beam to assign the material to it. Now the selection should have “1” in it, indicating that element 1 (the beam) is made of this material (“our silicon”).

5. In Physics we will set the boundary conditions.
a. In the left panel you can see that the default is "Free". For this, look (cf. click) at *Solid mechanics → free 1*. The second panel shows that faces 1 to 6 are free.
b. Now go to physics → boundaries → f ixed constraint. The beam turns gray. Select the first end face. Rotate the beam and select the other end face. The selection should now read 1, 6
c. Note the red symbol in *Solid mechanics → free 1*. Click on it to see that the free boundary conditions for face 1 and 6 show "overridden".

6. Select Mesh, Build Mesh. This divides the beam in tetrahedra for the calculation. These are the "Finite elements" that we are talking about.

7. Now we are all set to start the calculation.
a. Click study → compute
b. You now see deformed beam with colors indicating the total displacement**. View the mode from different angles. The frequency of 15 MHz is indicated in the caption. Verify that the mode is the first flexural (i.e., bending) mode in the vertical direction.
c. Click *Results → Mode shape (solid)*. Now we can select different eigenmodes. Pick another one and click Plot. That eigenmode is now shown.
d. Recall from the lecture: What is the ratio between the frequencies for vertical (z) and horizontal (y) flexural modes for a (tensionless) beam? Do the frequencies that you (well, COMSOL) calculated have the same ratio? (do not spend more than 5 min. on this part)
e. Go back to the calculated mode frequencies and their shape. Fill all the modes that you have found and identified at the correct location in the table below.

Mode	Longi. (MHz)		Tors. (MHz)		Flex. z (MHz)		Flex. y (MHz)	
	COMSOL	Anal.	COMSOL	Anal.	COMSOL	Anal.	COMSOL	Anal.
1		373.5		233.4		16.0		40.0
2		747.0		466.8		44.1		110.2
3		1120.4		700.3		86.4		216.1

The right side already contains the analytical results for the beam. Compare the analytical and your finite - element results.

** Note that silicon is a crystalline material that should be described by a full elasticity tensor for a cubic material. Read "What is the Young's modulus of Silicon", Hopcroft et al, J. Micromech. Syst. 2010 for details and the values of the elements of the elasticity and compliance tensor. Here we will simplify the problem by assuming that the material is isotropic with the abovementioned parameters.*
*** Recall that the magnitude of the eigenmodes is not fixed. Hence the fact that the simulation shows a crazy value for the maximum displacement of ~2.7 m for our nanobeam. This is something unique to eigenmodes. When calculating e.g. the static deflection induced by a load on the beam, the resulting displacement will be correct.*

f. Let's see if we can also see the longitudinal and torsional modes. Go to *study → eigenfrequency 1*, In “Search eigenfrequencies around” enter 300 MHz. Click Compute. Find the longitudinal and torsional mode and add these to the table. If you do not find the mode you look for, change the value or increase the number of eigenfrequencies to calculate. Enter in the table.
g. As you can see, all modes match well with the analytical calculations, except for the torsional mode. Any thoughts on why that could be?

Calculating the displacement of a SiN string under a load

1. Now we will look at the static deflection of a silicon nitride string with tension.

2. Save your previous work and make a new simulation. Select Stationary instead of Eigenmode.

3. Create a beam 100 um long, 500 nm wide, and 330 nm thick. Make sure to set the center to (0,0,0)

4. Now instead of Blank Material we use Browse materials. In the panel on the right type “silicon nitride“ and search. Select the hit Si3N4 from the MEMS toolbox. Click add to component and then Done. The material now appears in the left panel under materials. Go there and make sure that domain 1 is included

5. Set face 1 and 6 to the Fixed constraint boundary condition

6. Set face 3 (the bottom face) to Boundary load.

7. To specify the load, one can choose between e.g. Force per unit area and Total force. Choose Total force and enter -1e-8 N for the z component.

8. Build the Mesh and Compute the simulation

9. Now the plot shows the deformed shape (bending downward) but the colorscale is not what we want
a. Go to *Results → Stress (solid) → Volume 1*. Change Expression to “solid.disp” to show the total displacement, and click Plot.
b. We see that the maximum is about 70 nm.

10. Due to the large aspect ratio, the profile is not so well visible so let's make a cut line.
a. Go to Results → Cutline 3D
b. For the x coordinates of the two points use -50 um and +50 um. The y and z are OK (0 means that the cut will be the center of the string).
c. Click Plot. Something happens but you do not yet have the desired plot.
d. Choose Results → 1D plot group
e. Now in Data select Cut line 3D 1
f. In the menu item 1D plot group choose Line graph
g. Change expression to "w" to plot the z-displacement profile.
h. Now this is much clearer than the 3D plot and it shows the $x^2(L^2-x^2)$ shape

11. Now we want to find a more accurate value for the maximum displacement.
a. Go to Results → More derived Values → Volume minimum (note: w is negative)
b. Set selection to All domains, Expression to w.
c. Click evaluate. The value is 69.5 nm. Note that we have not included prestress in the model and this result is, thus, for bending rigidity only.

12. Silicon nitride typically has a lot of stress, and a typical value is σ = 800 MPa. Calculate the value of D/TL^2 for this situation, noting that $T = hw\sigma$ and $D = Eh^3w/12$. Does tension or bending rigidity dominate for this device?

13. How do we include the initial stress?
a. Click on:
b. *Solid Mechanics → Linear elastic material 1*
c. Type 800e6 in the 11 and 22 elements of the initial stress S0
d. Go to *Study 1 → Stationary* and check the box Include geometric nonlinearity. This is important as otherwise the stress not completely taken into account.
e. Rerun the simulation
f. Check the shape. What is different? What is now the largest vertical displacement?

14. Note that the stress is not the value that we entered. This is because the stress relaxes in the y direction (remember that $\sigma_{yy} = 0$ for the thin beam we discussed in the lecture?). We are going to make a 2D plot to see this.

a. Results → cut plane
b. Set the x value to 25 um
c. Results → add 2D plot group
d. 2D plot group 3 → Surface
e. Set Dataset to the cut plane that you just made and Expression to "solid.sl11". This will plot the stress σ_{xx}. Note that there is an average value and a linear gradient in the z direction. Remember the parametrization of the beam $u_x = z\, du/dx$? This gave us a strain and σ_{xx} that varies linearly with z. To visualize this, replot the surface but now with the Expression "solid.sl11 - XXX" where XXX is the value of the average that you saw before.

To calculate the average stress in the xx direction, choose Results → More derived values → Surface averaging. Now select the cut plane and set the expression to “solid.sl11”.

f. Note that the value of 618 MPa is lower than the 800 MPa that we started with.
This because σyy relaxed to 0-ish, indicating shrinking in that direction. The Poisson ratio converts this into an expansion in the x direction reducing the stress there.
g. Some more simulations are summarized in the table. Do you understand the results?

Force (nN)	Initial stress (MPa)	Max. displ. (nm)	σ_{xx} (MPa)
-10	0	-68	0.3
-10	800	-1.28	618
-10	1000	-1.10	772
-100	1000	-9.3	772
-1000	1000	-91.7	773
-10000	1000	-863	821

15. Save your work.

4. **The outcome of the tutorial: what will the students learn after attending it?**

Participants will learn to navigate the user interface, create geometries, choose materials, apply meshes, and calculate properties of nanoscale structures such as a Si nanobeam and a SiN nanostring. By the end of the tutorial, participants will be equipped to apply COMSOL in their studies and research of (nano)mechanics. The tutorial will also advance their understanding of nanoscale mechanical systems.

5. **Keywords for which fields of physics this tutorial might be relevant. You might have mentioned one or two in the track field, but if you feel like it is relevant for the other disciplines, feel free to mention it here.**

Computer simulations, mechanics, nanoscience