Lecture: P1_Wk5_L1

Force-Distance Simulations with VEDA

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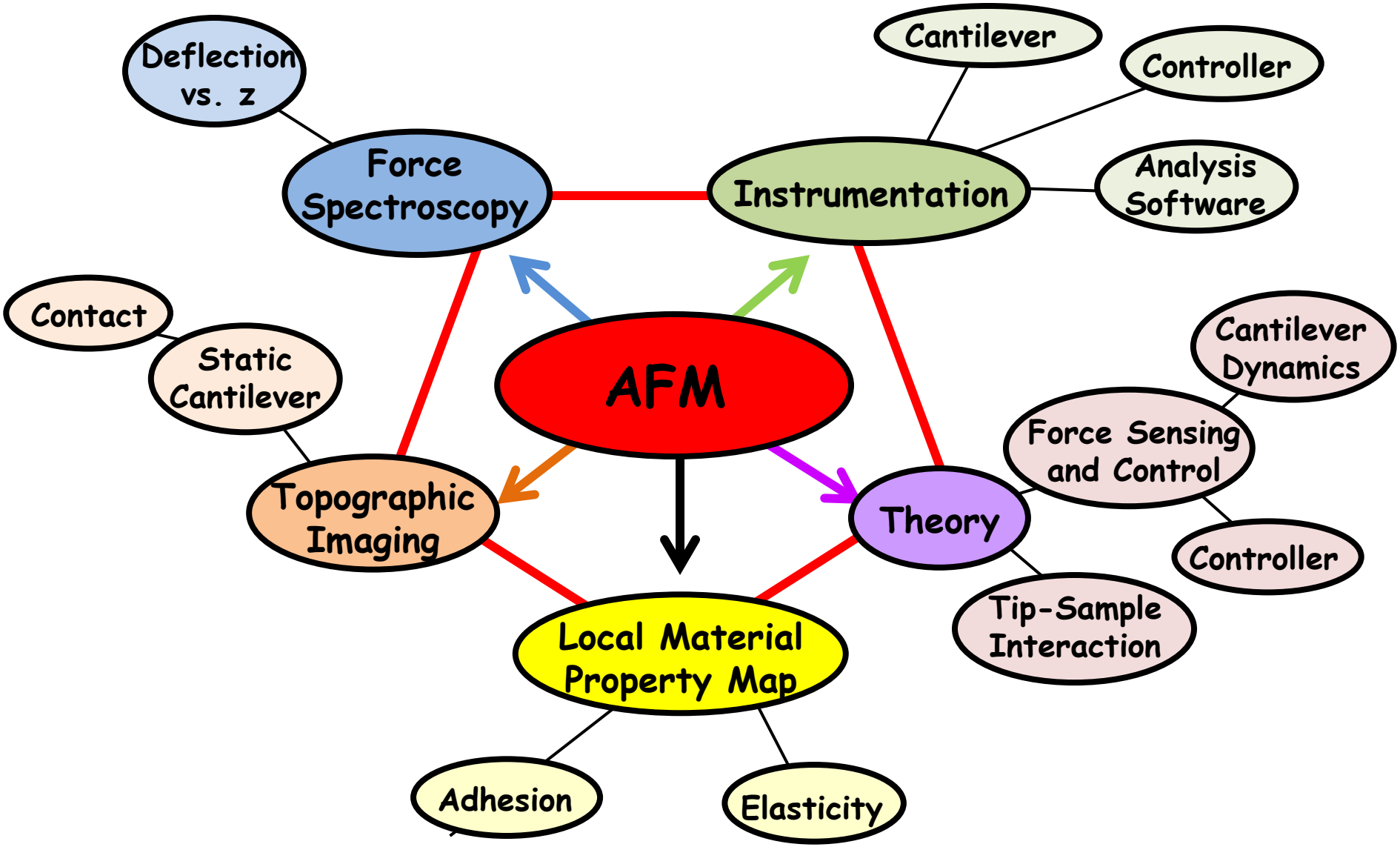
for VEDA overview: Rev. Sci. Instrum. 83, 013702 (2012)
(you must have Java version 1.4 or later installed on your machine and enabled in your web browser)

PURDUE UNIVERSITY


Deflection vs. z
Force Spectroscopy
Cantilever
Controller
Instrumentation
Analysis Software
Contact
Static Cantilever
AFM
Topographic Imaging
Cantilever Dynamics
Force Sensing and Control
Theory
Controller
Tip-Sample Interaction
Local Material Property Map
Adhesion
Elasticity

First - A Few Comments

It is more effective to spend time and learn VEDA than to write the equivalent software yourself.

You can improve your efficiency on an AFM instrument by first running realistic simulations of experiments that you might perform.

If you see an empty graph after a simulation, use the Result menu in the Simulate tab and select ErrorMessage. Usually a helpful hint will appear.

If an input window happens to require two input values, make sure they are **comma separated**.

If a plot doesn't make sense, try a different value for k, the cantilever spring constant. Results of almost any VEDA simulation should change with k.

For initial use of a tool, choose the input default values and make sure you understand the resulting plot(s) before tailoring to your application.

Sometimes, a simulation will "time out" before it begins. Usually, this means the feedback parameters are set too high.

If you do not understand requested parameters, check out the complete VEDA manual which is currently located at nanohub.org/resources/adac/supporting docs

If you have a reasonably reliable internet connection, the **longest** time required for an approach curve simulation is about 1 minute of real time.

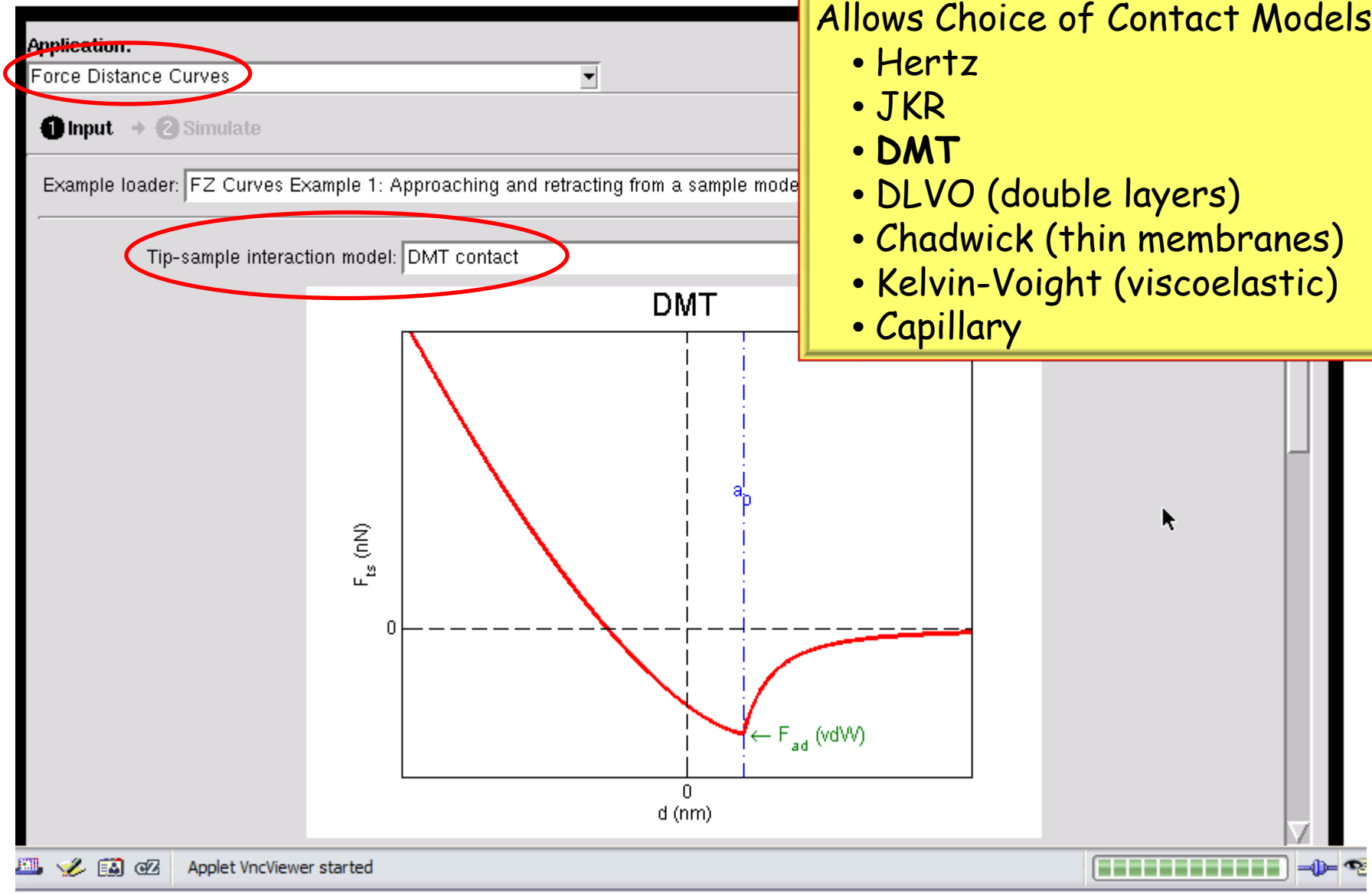
Whether you perform an approach or retract simulation depends on the initial and final z separation that you specify. For example:

- Initial z separation=+6 nm, Final z separation= -6 nm: **approach**
- Initial z separation=-6 nm, Final z separation= +6 nm: **withdraw**

Force-Distance Simulations using VEDA

1. Go to the NanoHub at http://nanohub.org/ and login to your account
2. Locate the VEDA software and launch the tool
3. **OR** access VEDA from the NanoHUB-U course page
4. Select the "Force Distance Curves" application

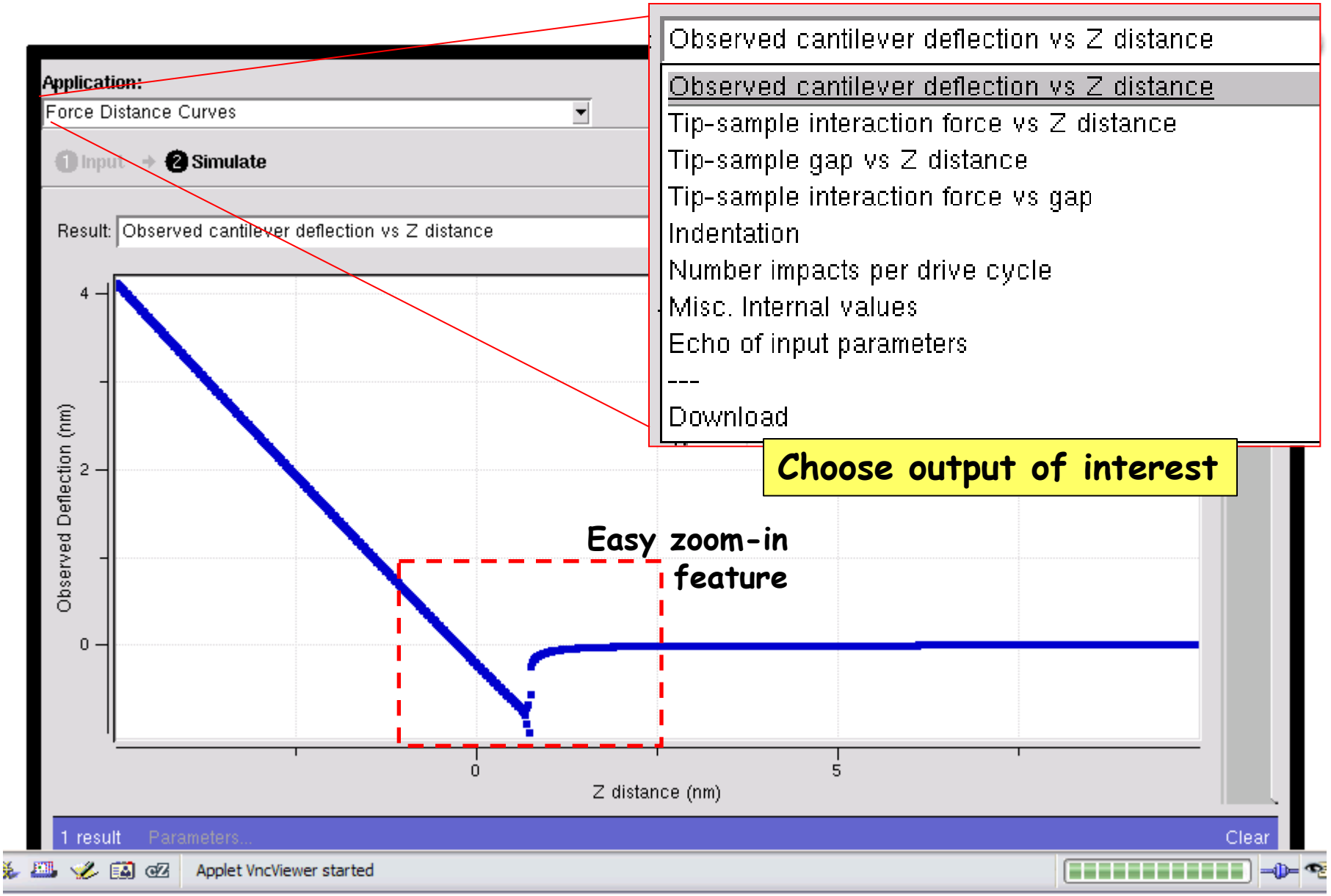
The Force Distance Module



Allows Choice of Contact Models

- Hertz
- JKR
- **DMT**
- DLVO (double layers)
- Chadwick (thin membranes)
- Kelvin-Voight (viscoelastic)
- Capillary

Many Simulations are Possible



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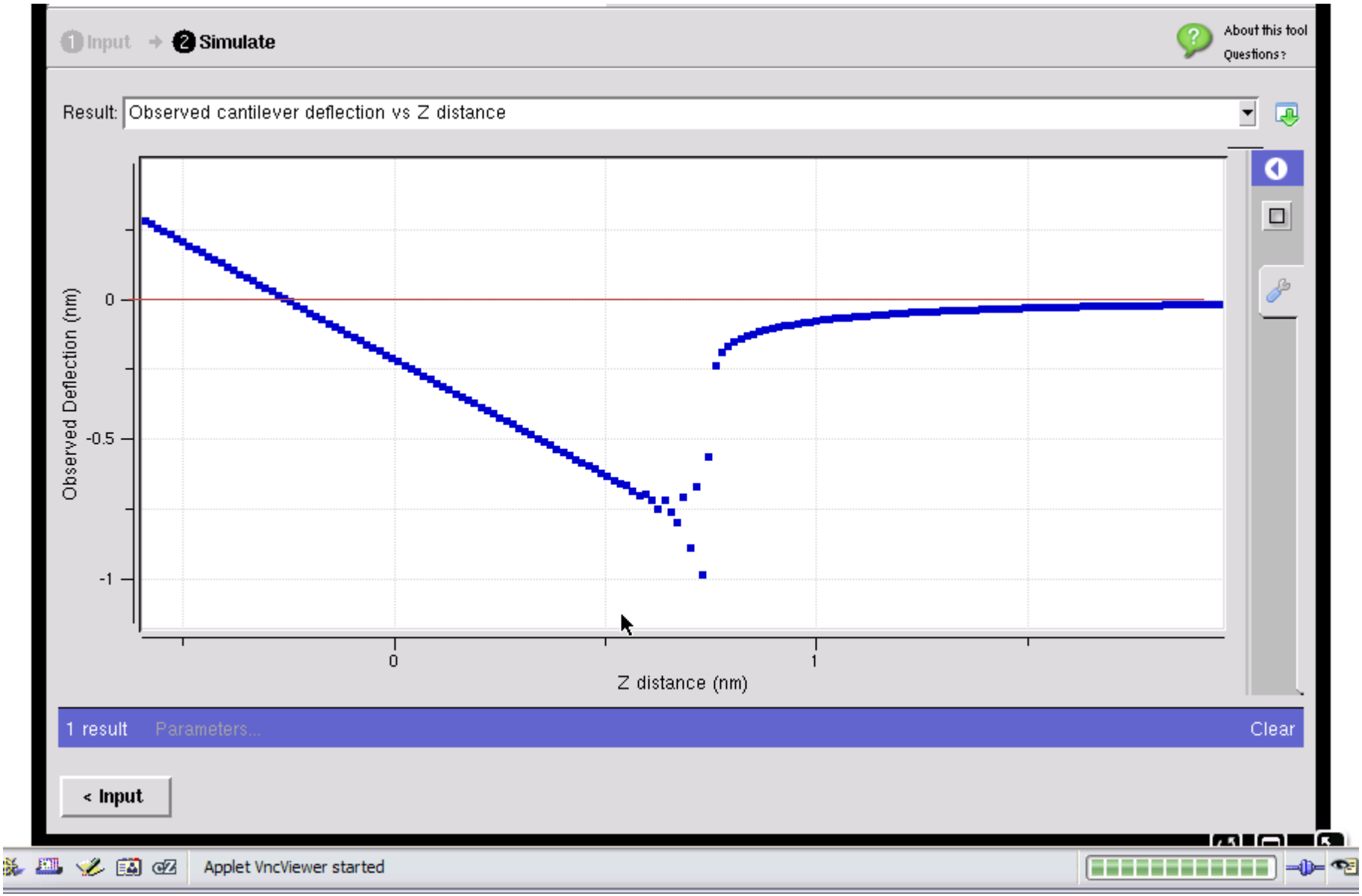
Simulation results - magnified



Example 1:

You have two samples A and B, having a Young's modulus of 1 GPa and 0.1 GPa respectively.

a) Perform F-z simulation starting from a z-distance of 5nm and approach to a z-distance of -5nm.

b) Compare to an infinitely hard sample.

c) What is the indentation as a function of z?

Except for substrate E, use the default values provided by VEDA (DMT tip-sample interaction).

First, a copy of the Echo Input File for the first simulation. Most of the parameters are defaults. Many of the listed parameters are not used in this simple example.

exc_choice = 1
operating mode 1 fexcite 3 numModes
1
LockInTC (us) 0.000000000000000E+000
LockInOrder 0
mtip 0
omegad 44
Ainitial = 1
AprchS 200
gamma_drag 3.77e-06
omega = 44
Keq = 5
Chi = autocalc
Q = 33
Rtip = 10
Etip = 130
Poisson_tip = 0.3
mat properties for: input.phase(ts)
want WLC F
kts_R 10
kts_A 10
Fadhesion 1.4167
A_hamaker 3.4E-20
fts_model 3
want tip squeeze F
want oscillatory F
want hydration F
want v_ie F
electrostatic theta tip 10
electrostatic theta lever 10
electrostatic height 10
electrostatic length 100
electrostatic width 30
VEchoice 1
WantCapAd F
Esample 1
Poisson_sample 0.3
KD 0.001
epsilon 80
sigmat -0.0025
sigmas -0.032
hs 6
want presiach F
Zrange 2
Z0 5
Zf -5
plotpnts 1000 numincycle 1000
transient_allowance

k_{cant} = 5 N/m

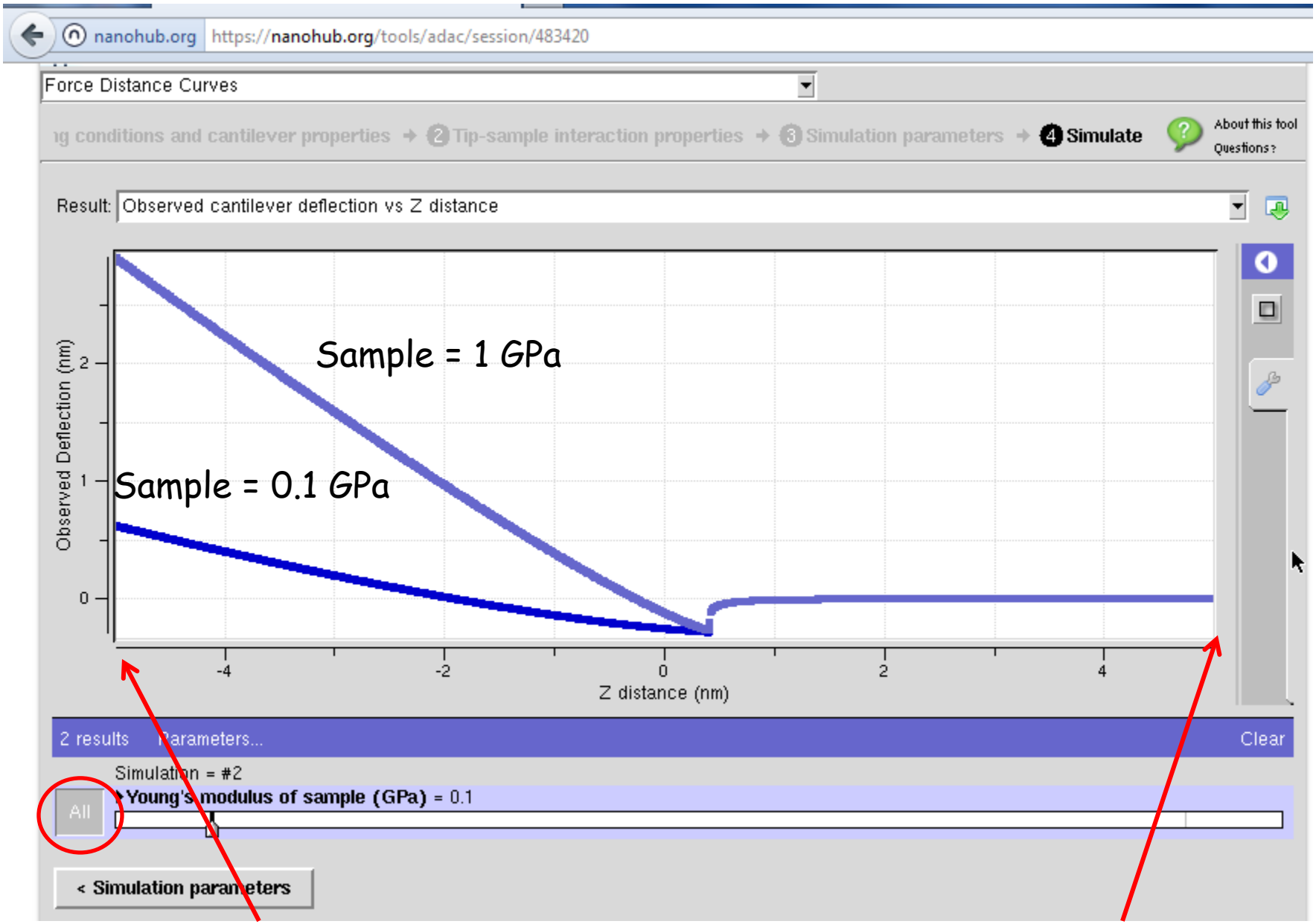
R_{tip} = 10 nm

E_{tip} = 130 GPa

E_{sample} = 1 GPa

-5 nm < z < +5 nm

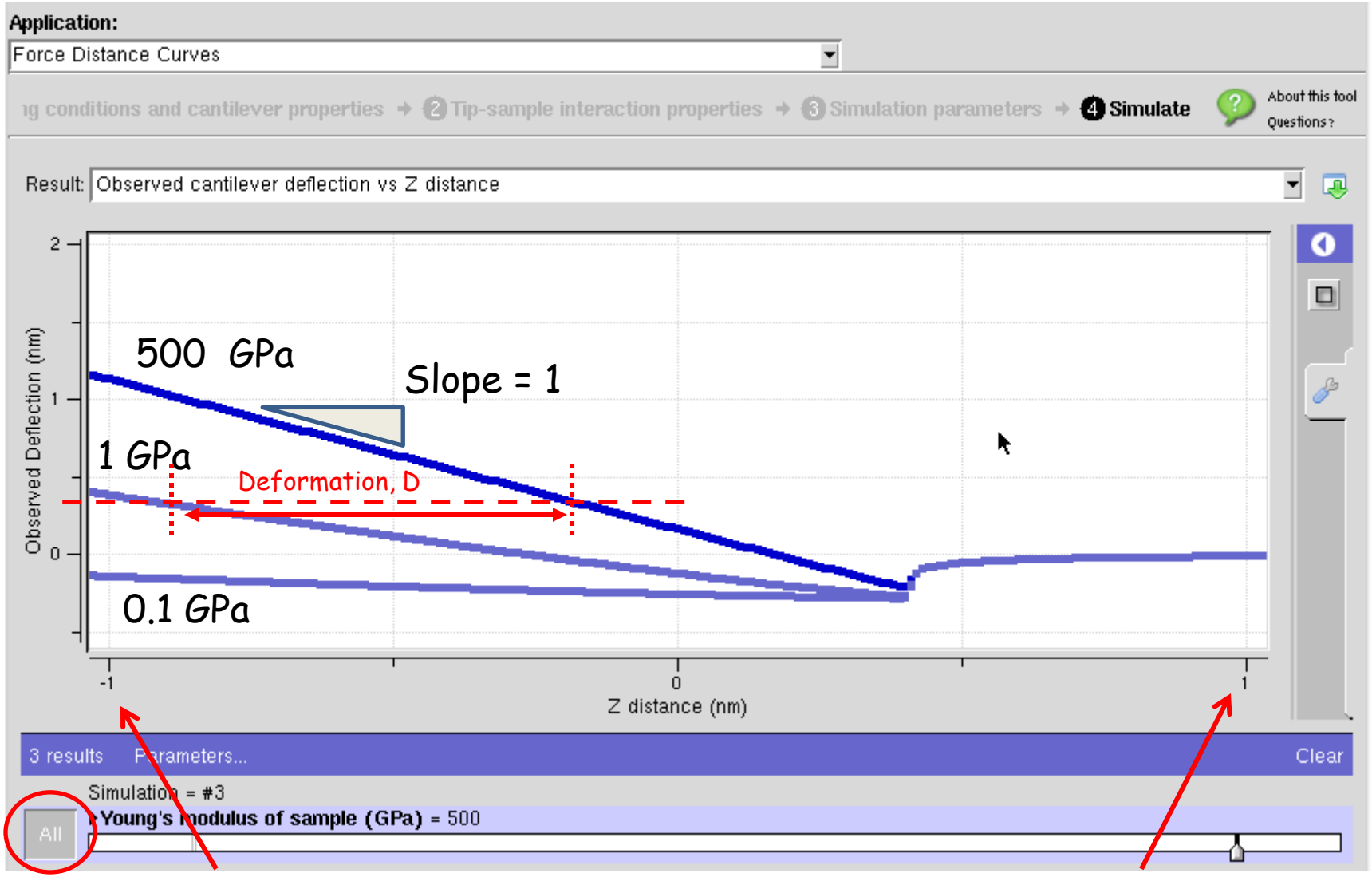
Results



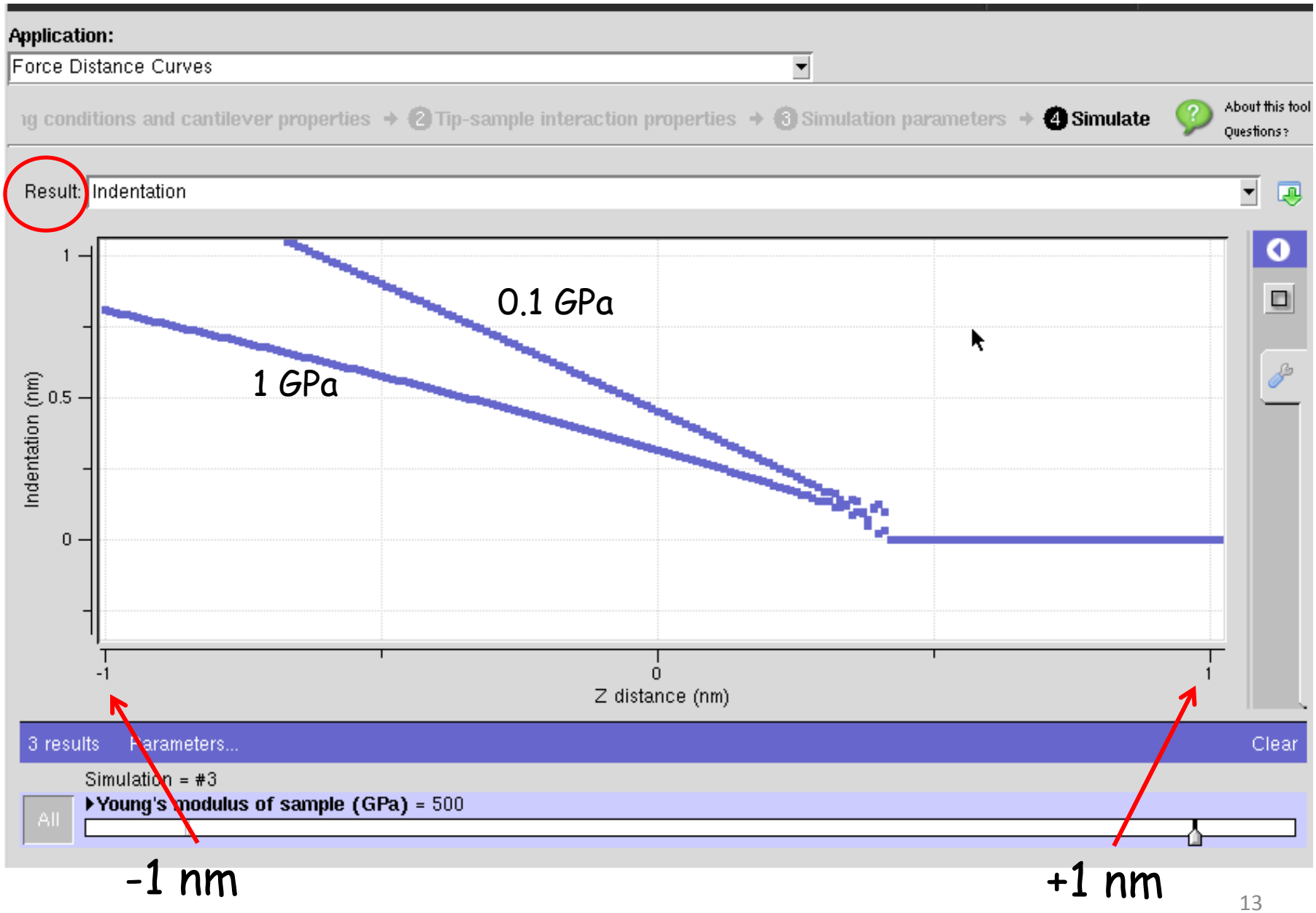
-5 nm

+5 nm

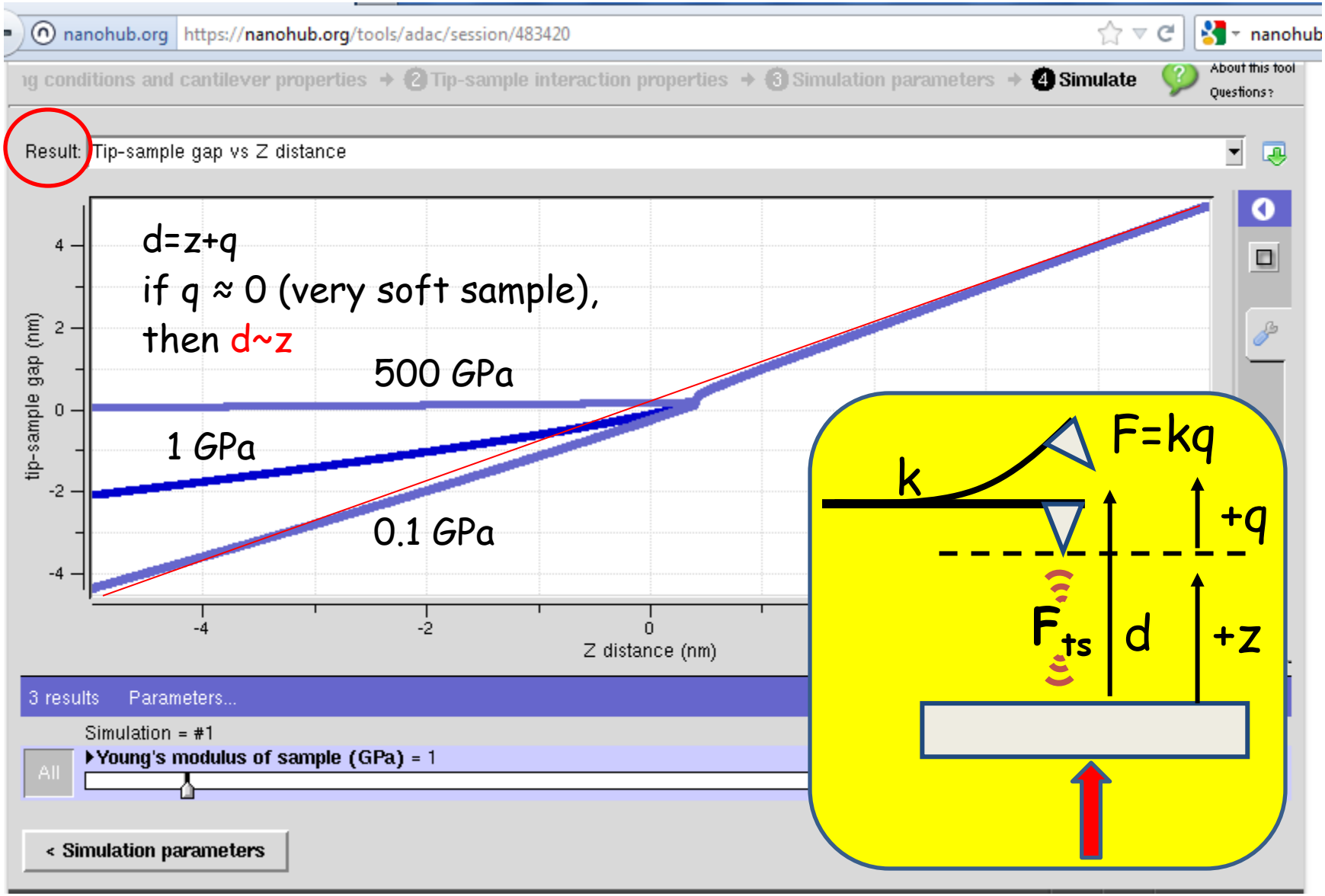
Magnified near Jump-to-Contact; include infinitely hard sample



Indentation Plot



Tip-Sample Gap



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Example 2:

You have a very soft sample with an elastic modulus of 0.5 GPa. It is known that a force of 500 pN or higher will reversibly damage the sample. You have the choice of two cantilevers with stiffness values 0.1 N/m and 1 N/m.

a) At what z-distances will these two cantilevers jump to contact?

b) Which cantilever would be the best if you wanted to investigate the relevant tip-sample forces when d= +0.9 nm?

c) Using the 1 N/m cantilever, estimate the maximum Z value permissible without causing permanent damage?

For all other parameters, use the default values provided by VEDA (use the DMT tip-sample interaction).

See Appendix

Up Next: Force-Distance Simulations using the JKR Model; Investigating the effect of tip radius; Hertz Model

Appendix

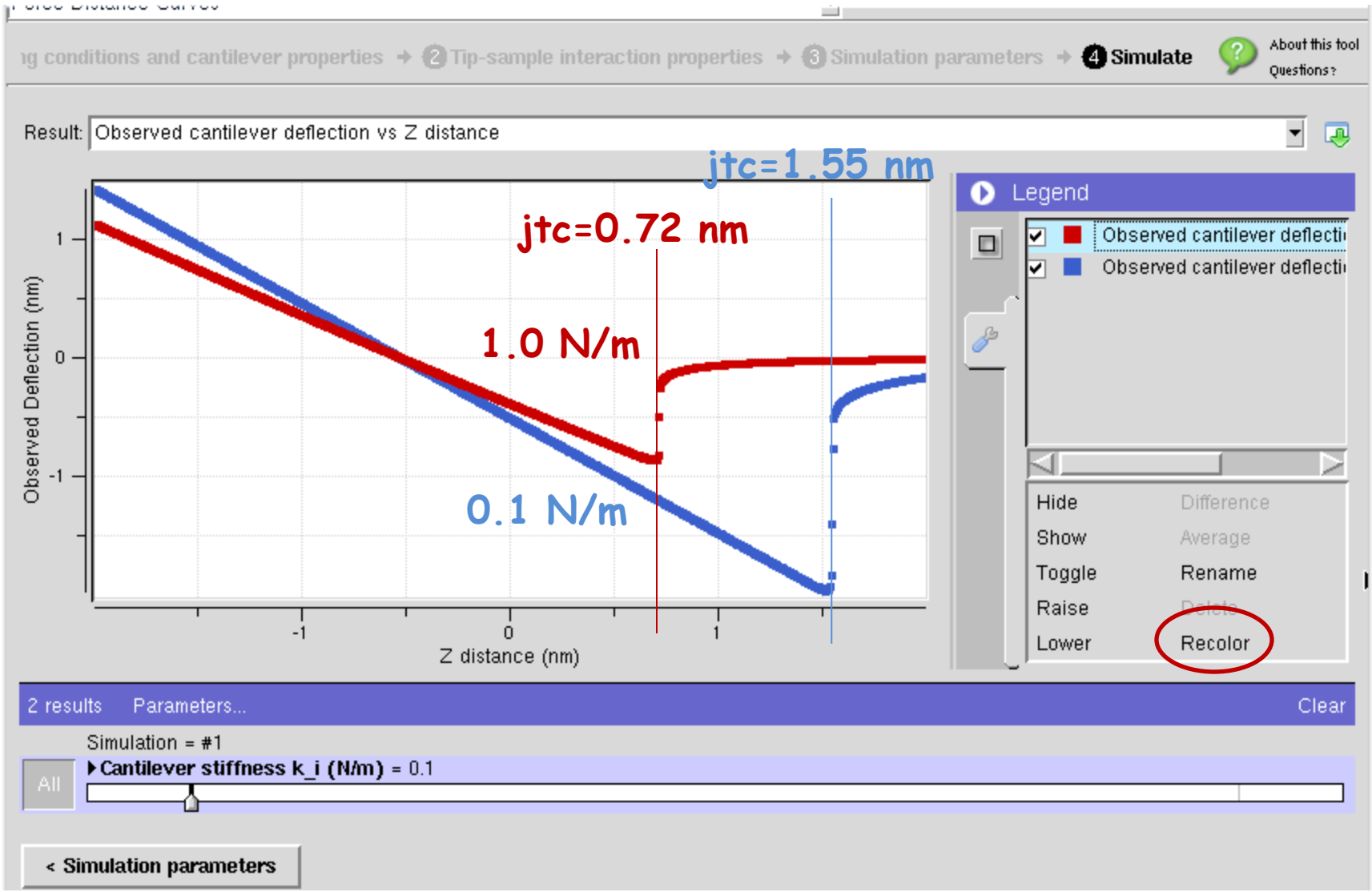
Example 2: Use the DMT Contact Model

First, a copy of the Echo Input File for the first simulation. Most of the parameters are defaults. Many of the listed parameters are not used in this simple example.

exc_choice = 1
operating mode 1 fexcite 3 numModes 1
LockInTC (us) 0.000000000000000E+000
LockInOrder 0
mtip 0
omegad 44
Ainitial = 1
AprchS 200
gamma_drag 3.77e-06
omega = 44
Keq = 1 k_{cant} =1 N/m
Chi = autocalc
Q = 33
Rtip = 10 R_{tip} = 10 nm
Etip = 130
Poisson_tip = 0.3
mat properties for: input.phase(ts)
want WLC F
kts_R 10
kts_A 10
Fadhesion 1.4167
A_hamaker 3.4E-20
fts_model 3
want tip squeeze F
want oscillatory F
want hydration F
want v_ie F
electrostatic theta tip 10
electrostatic theta lever 10
electrostatic height 10
electrostatic length 100
electrostatic width 30
VEchoice 1
WantCapAd F
Esample 0.5 E_{sample} = 0.5 GPa
Poisson_sample 0.3
KD 0.001
epsilon 80
sigmat -0.0025
sigmas -0.032
hs 6
want presiach F
Zrange 2
Z0 2
Zf -2 -2 nm < z < +2 nm
plotpnts 1000 numincycle 1000
transient_allowance

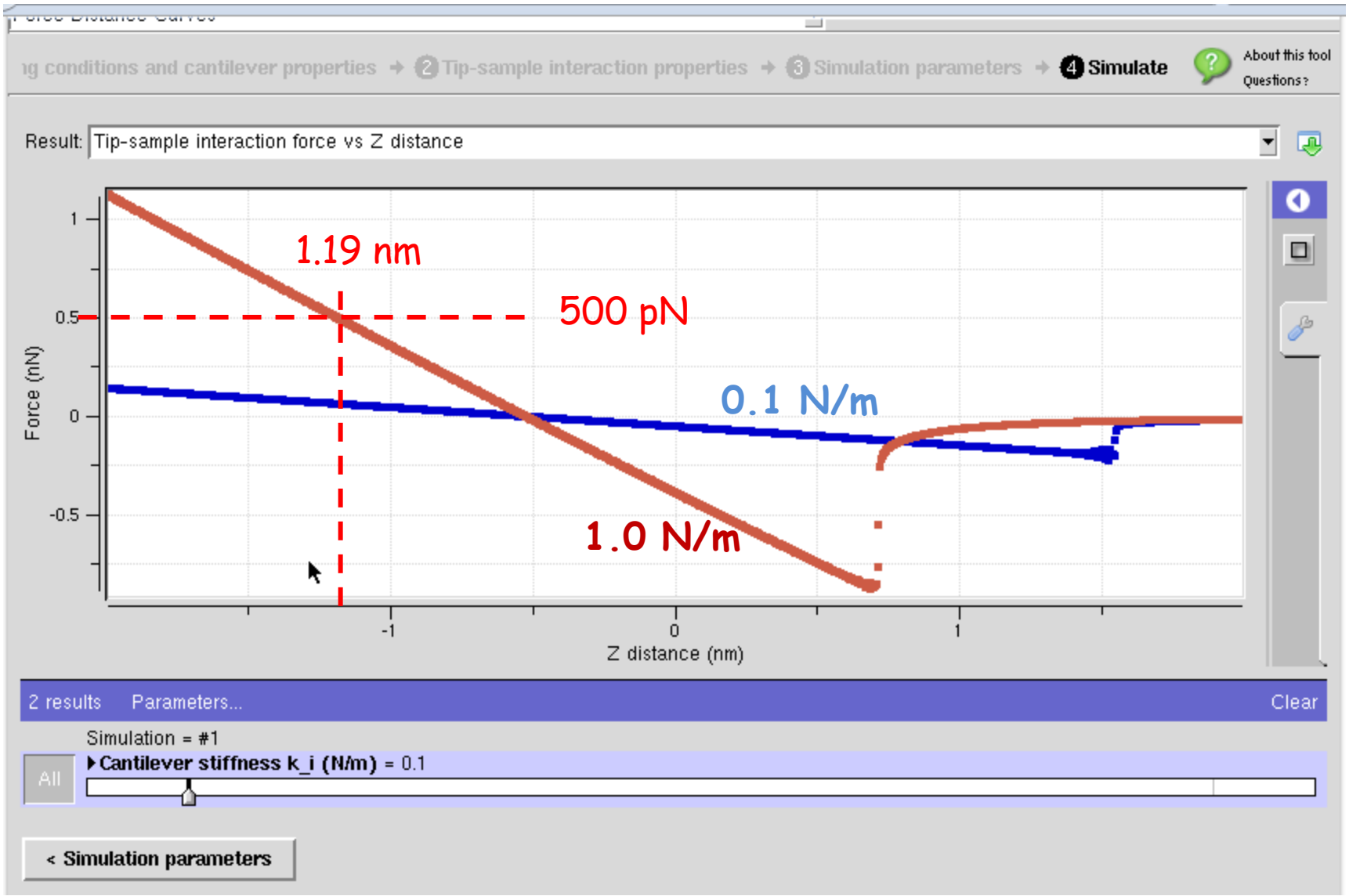
Cantilever Deflection vs. z

(measure jump to contact distances)



Force vs. z

(sample damage will result if |z|>1.19 nm for 1.0 N/m cantilever)



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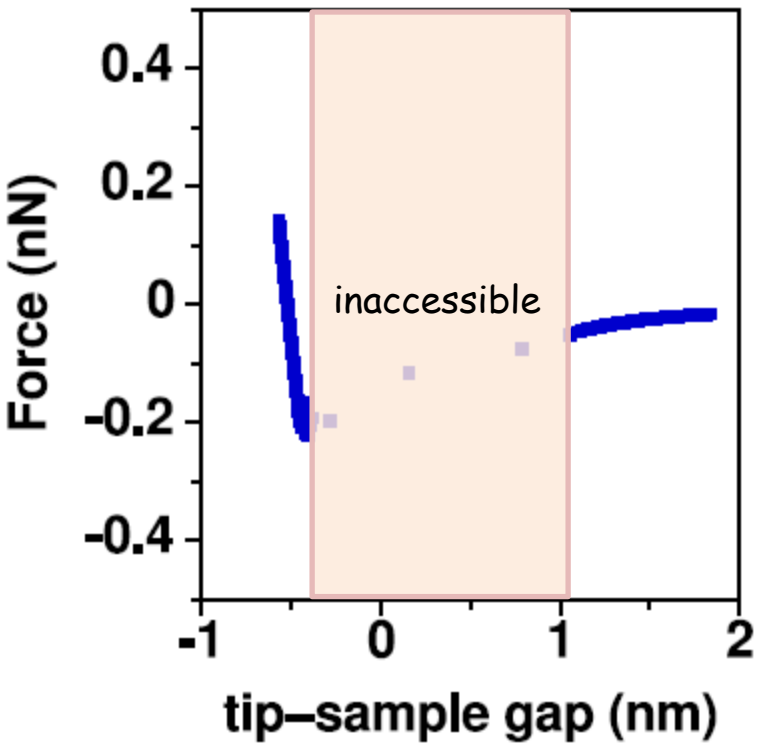
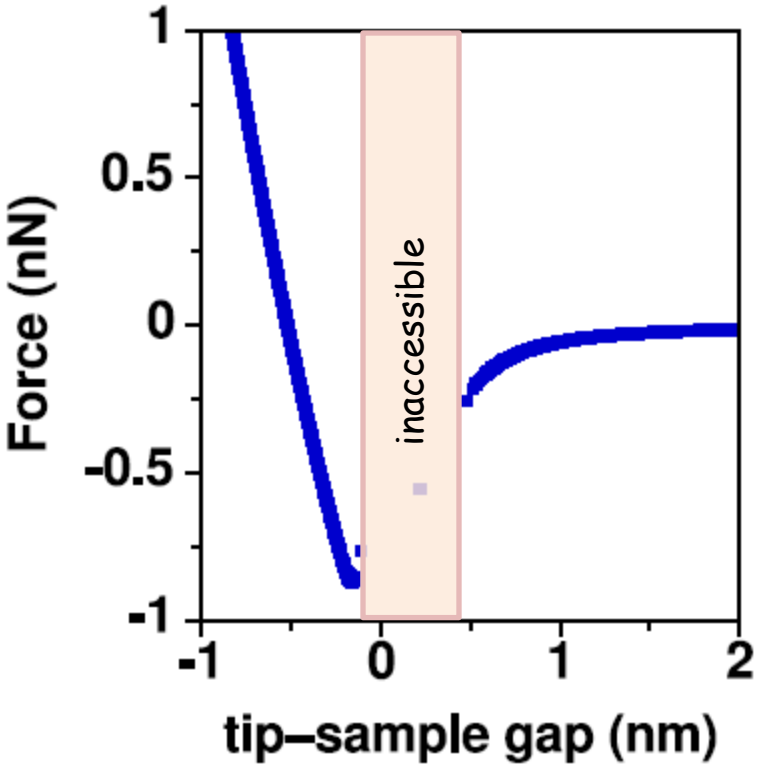
Force vs. Tip-Sample Gap

(example of publication quality graphs from VEDA)

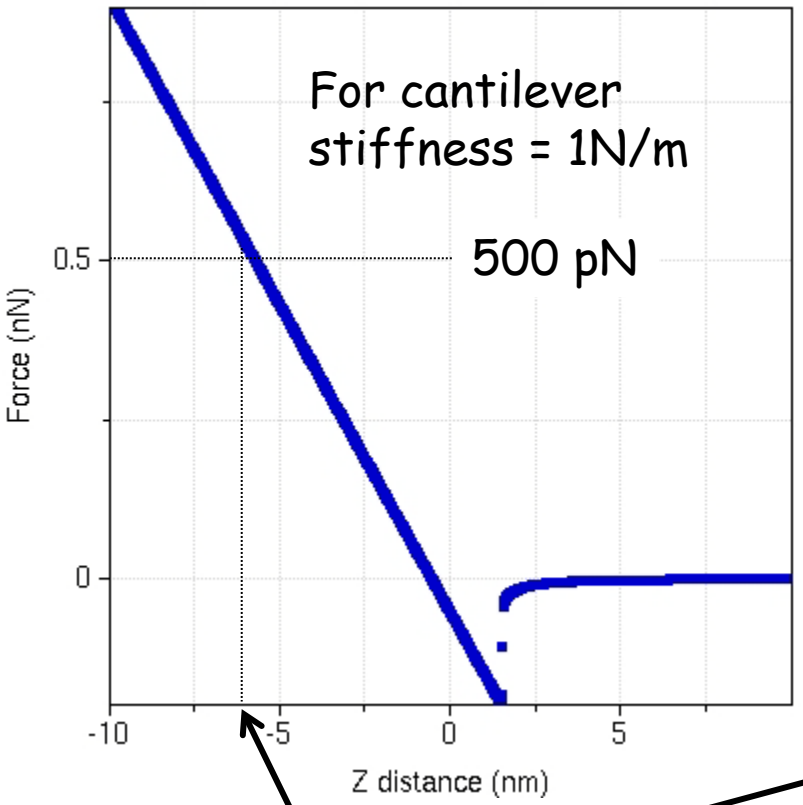
k=0.1 N/m

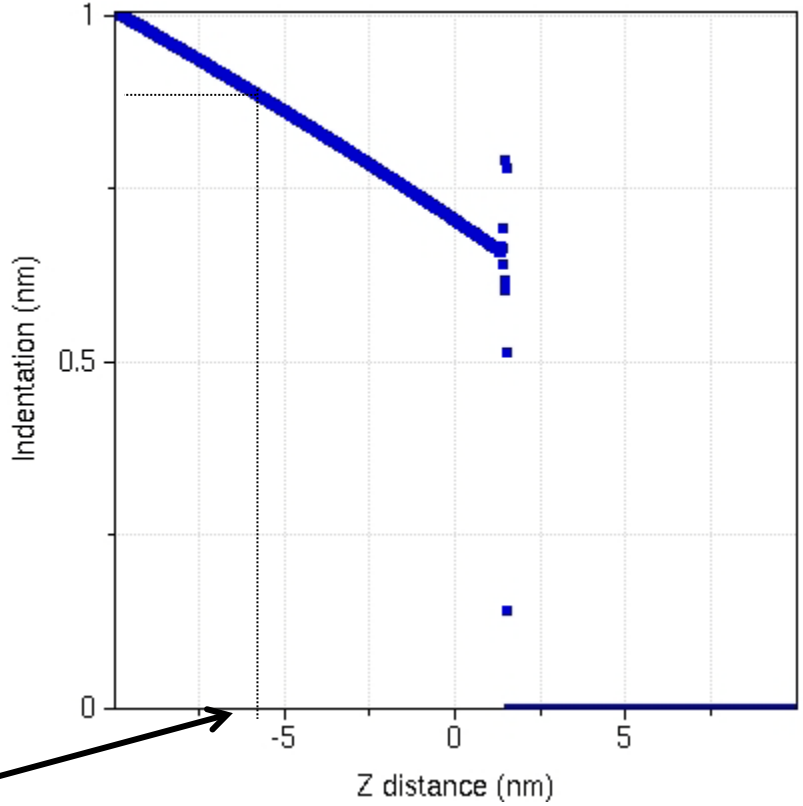


k=1.0 N/m



If you were to run an experiment, approximately when would you stop the z-approach to avoid damage to the sample?



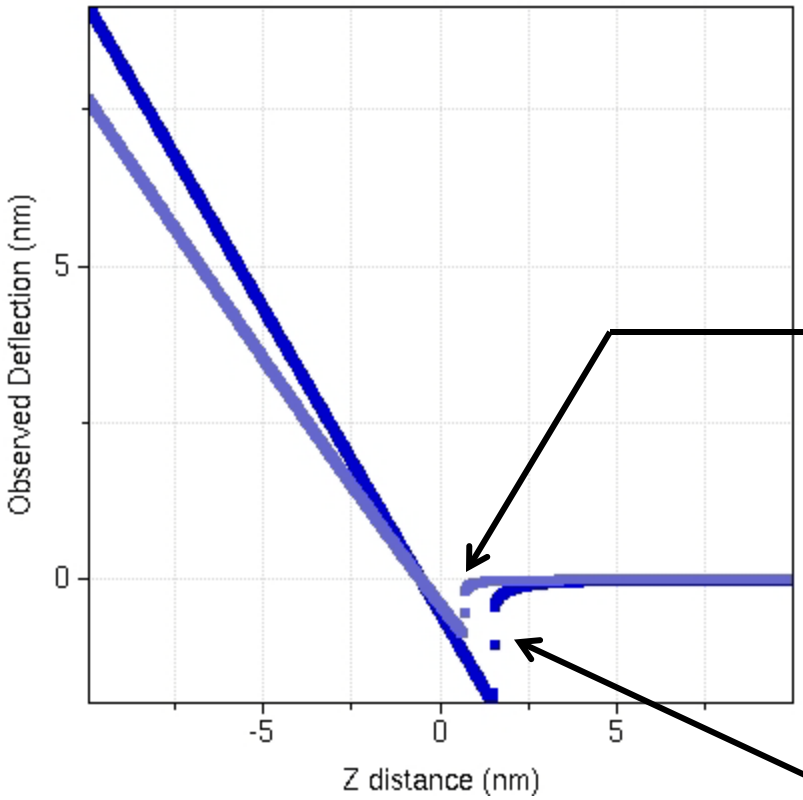


Max. permissible z distance is about -5.7nm (for F = 500 pN)

Max. indentation for z=-5.7nm is about 0.88nm

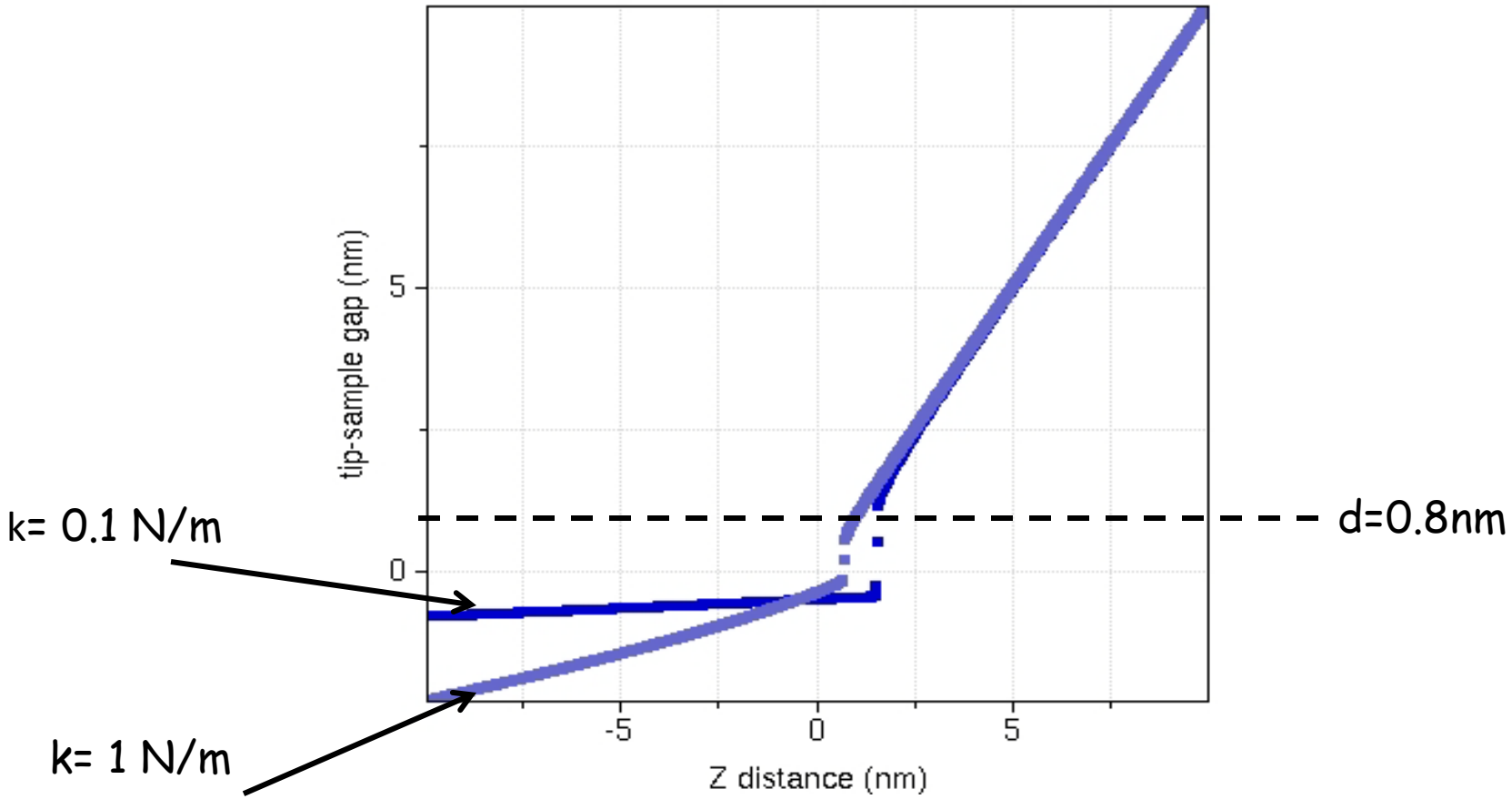
If you choose a different cantilever stiffness, the z-distance value (for F =500 pN) will change.

b)



The respective x-axis values give the distances at which the snap-in occurs.

Note: other graphs including d-z and F-z can also be used to determine the z-distance at which the snap-in occurs.



- The cantilever which has a stiffness of k=1 N/m must be selected to study the force at d=0.8 nm since the other cantilever (k=0.1 N/m) will snap-in at this d value.

- In general, softer cantilevers snap-in at larger d-values.