

Lecture: P1_Wk5_L2

Force-Distance Simulations with VEDA:

JKR Model

Tip radius

Hertz Model

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for VEDA overview: Rev. Sci. Instrum. 83, 013702 (2012).

for VEDA Manual:

https://nanohub.org/resources/14230/download/VEDA_Manual.pdf

VEDA has a number of examples preloaded

The screenshot displays the VEDA 2.0 (Virtual Environment for Dynamic AFM) interface. At the top, there are buttons for 'Terminate' and 'Keep for later'. Below the title bar, the 'Application:' dropdown menu is set to 'Force Distance Curves'. A navigation bar shows three steps: '1 Operating conditions and cantilever properties', '2 Tip-sample interaction properties', and '3 Simulation parameters'. An 'About this tool Questions?' link is also present. The 'Example loader:' dropdown menu is open, showing two options: 'FZ Curves Example 1: Approaching and retracting from a sample modeled using DMT contact' and 'FZ Curves Example 2: Approaching and retracting from a sample modeled using JKR contact'. Below the dropdown, various simulation parameters are listed with input fields and checkboxes.

Application: Force Distance Curves

1 Operating conditions and cantilever properties → 2 Tip-sample interaction properties → 3 Simulation parameters → About this tool Questions?

Example loader: FZ Curves Example 1: Approaching and retracting from a sample modeled using DMT contact
FZ Curves Example 2: Approaching and retracting from a sample modeled using JKR contact

Auto calculate stiffnesses k_i ($i>1$)?: no

Cantilever stiffness k_i (N/m): 5

Quality factor(s): 33

Auto calculate ω_i ($i>1$)?: no

Natural frequency f_i (kHz): 44

Tip mass: 0

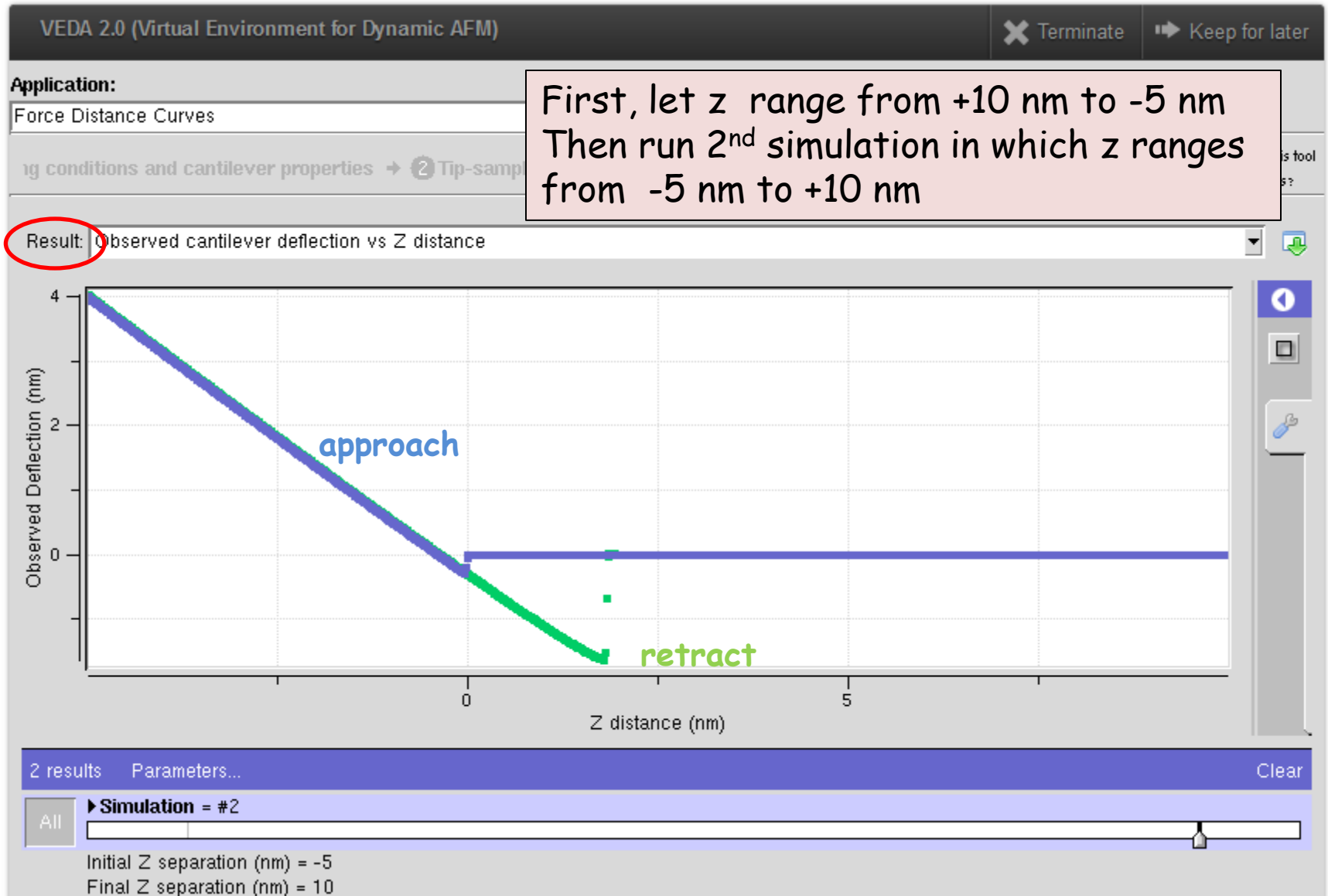
Z approach/retract speed (nm/s): 200

gamma (Z drag): 3.77e-06

Initial Z separation (nm): 10

Final Z separation (nm): 0

JKR approach and retract curves

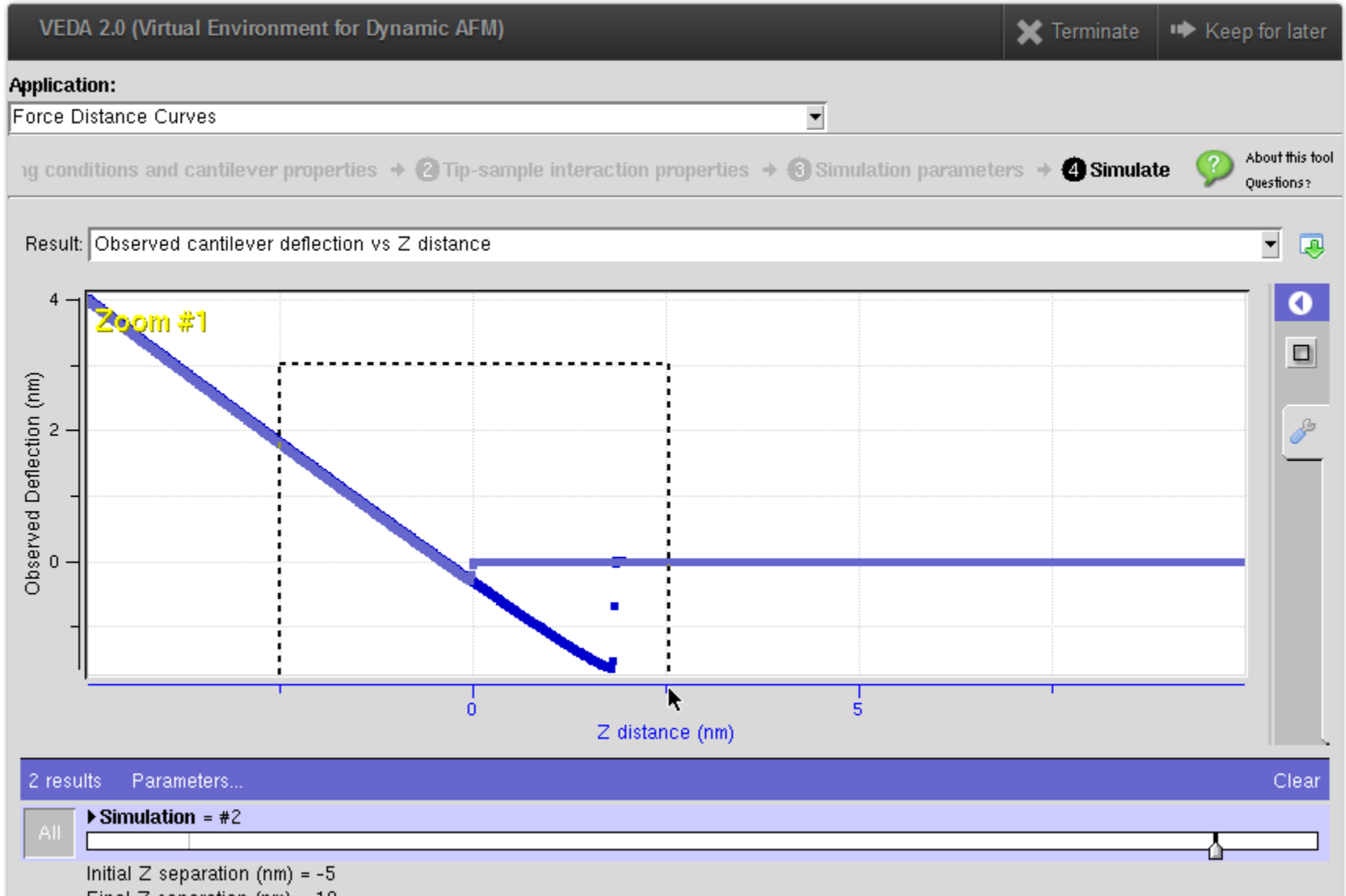


$$k_{\text{tip}} = 0.87 \text{ N/m}$$

$$R_{\text{tip}} = 10 \text{ nm}$$

$$E_{\text{sample}} = 1 \text{ GPa}$$

Zoom in on features of interest



Plot after enlarging



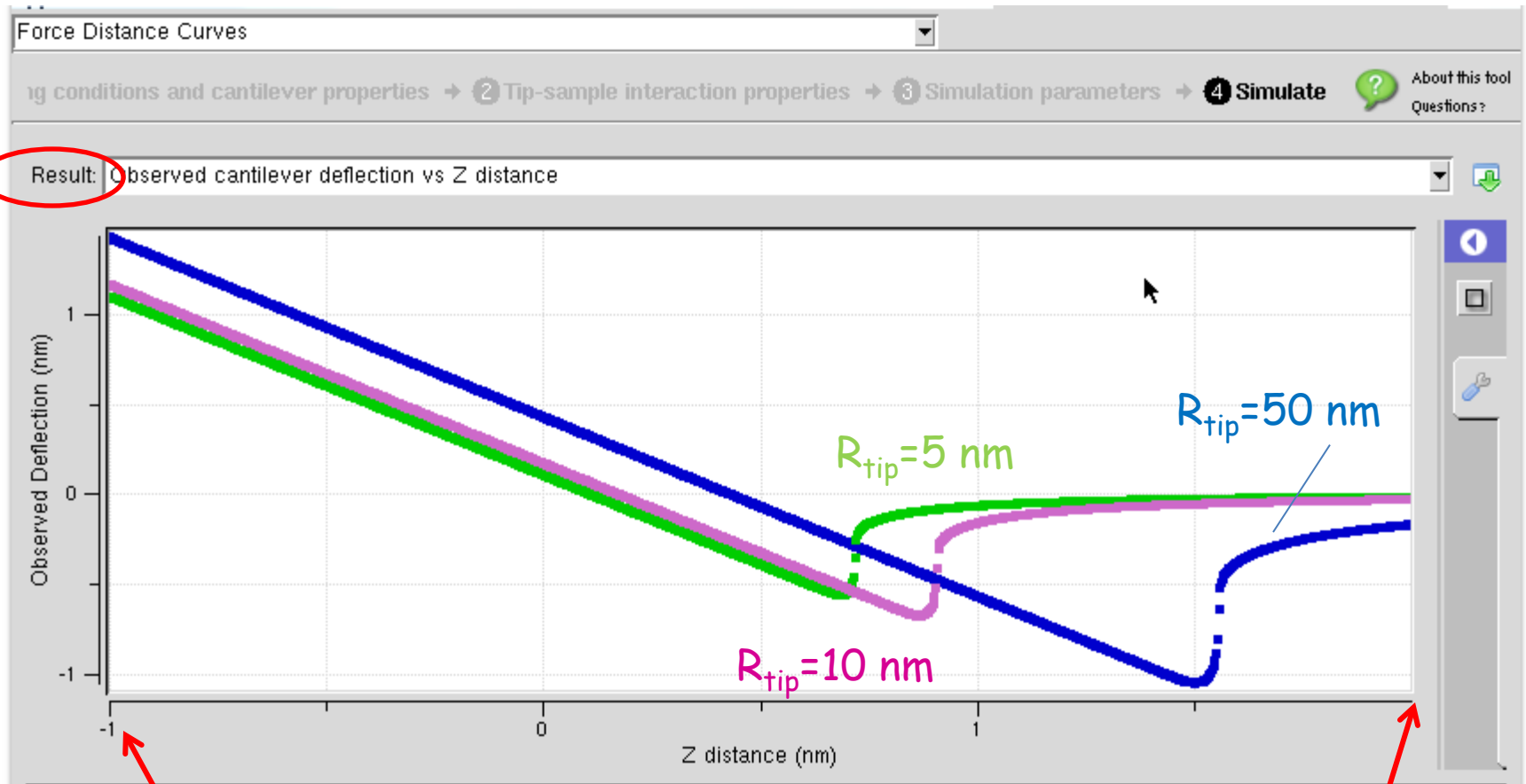
Example 1:

You have a sample with a Young's modulus of 200 GPa. Assume the DMT model for tip-sample interaction. Use a cantilever with a 0.5 N/m spring constant.

- a) Perform F-z simulation starting from a z-distance of 2 nm and approach until a z-distance of -1 nm is reached.
- b) How does the tip radius effect the force-distance data? Investigate $R_{\text{tip}} = 5 \text{ nm}$, 10 nm and 50 nm.

Use the default values provided by VEDA for all other parameters.

Cantilever Deflection vs. z



-1 nm

+2 nm

Example 2:

You have a sample having a Young's modulus of 500 GPa. Assume the Hertz model for tip-sample interaction and investigate the effect of capillary forces. Use a cantilever with a 0.5 N/m spring constant.

- a) Perform F-z simulation starting from a z-distance of 5 nm and approach to a z-distance of -2 nm.
- b) For the capillary force, choose a pull-off distance of $d=0.6$ nm.
- c) Simulate two different energy dissipations of 1 and 2 eV. This is the energy dissipated on withdrawal.

Use the default values provided by VEDA for other parameters.

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) 0.0000000000000000E+000
LockInOrder 0
mtip 0
omegad 44
Ainitial = 1
AprchS 200
gamma_drag 3.77e-06
omega = 44
Keq = .5  $k_{cant} = 5 \text{ N/m}$ 
Chi = autocalc
O = 33
Rtip = 10  $R_{tip} = 10 \text{ nm}$ 
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 2
want tip squeeze F
want oscillatory F
want hydration F
```

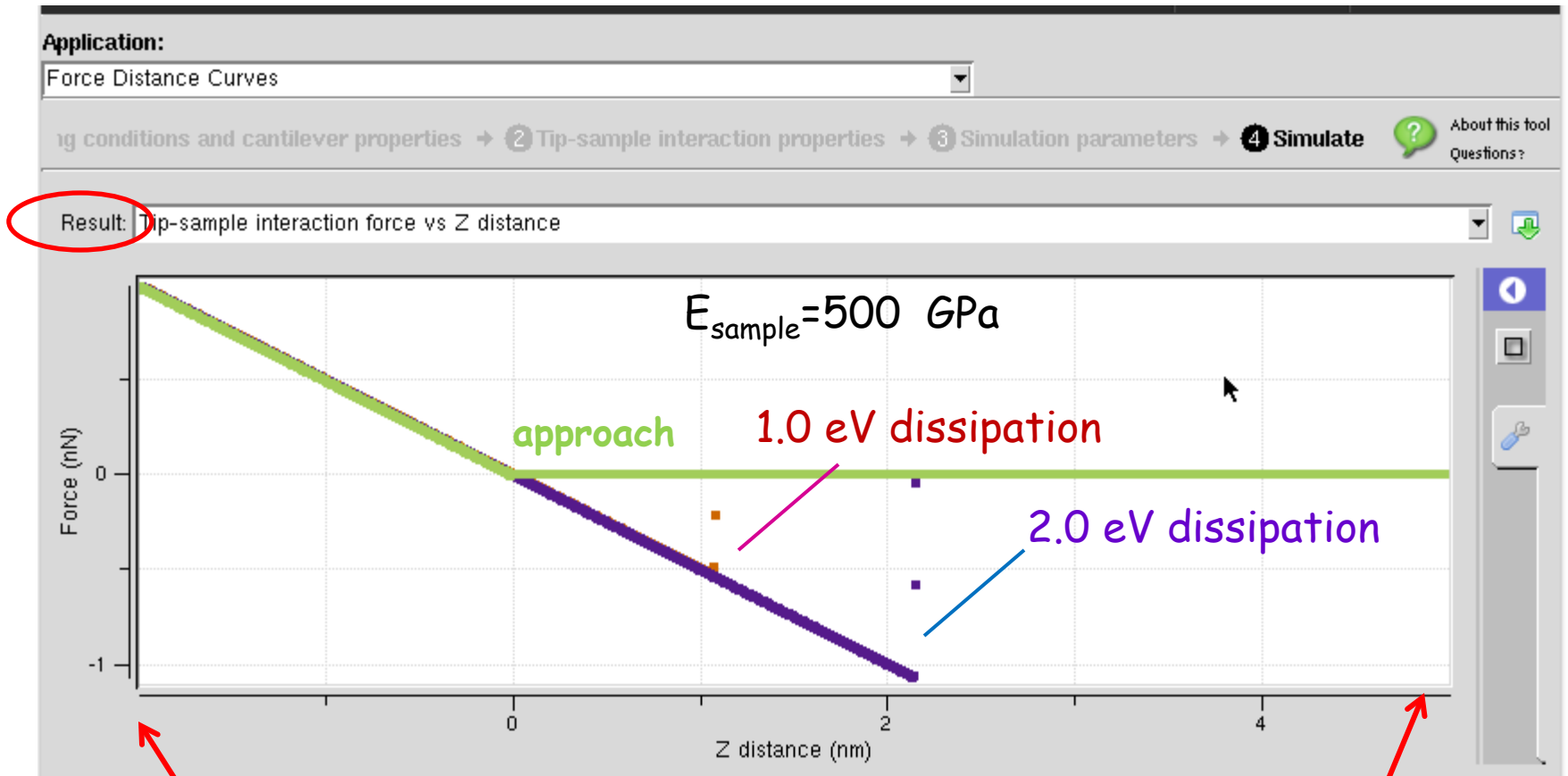
```
want v_ie F
electrostatic theta tip 10
electrostatic theta lever 10
electrostatic height 10
electrostatic length 100
electrostatic width 30
VEchoice 1
WantCapAd T
D_0 0.6
deltaE 1
Esample 500  $E_{sample} = 500 \text{ GPa}$ 
Poisson_sample 0.3
KD 0.001
epsilon 80
sigmat -0.0025
sigmas -0.032
hs 6
want presiach F
Zrange 2
Z0 -2  $-2 \text{ nm} < z < +5 \text{ nm}$ 
Zf 5
plotpnts 1000 numincycle 1000
transient_allowance
```

Capillary adhesion

$E_{sample} = 500 \text{ GPa}$

$-2 \text{ nm} < z < +5 \text{ nm}$

Force vs. z



-2 nm

+5 nm

capillary force observed upon retraction

Does the observed cantilever deflection depend on elastic modulus of the sample?

(pick 2 eV dissipation, vary E_{sample})
plot approach curves

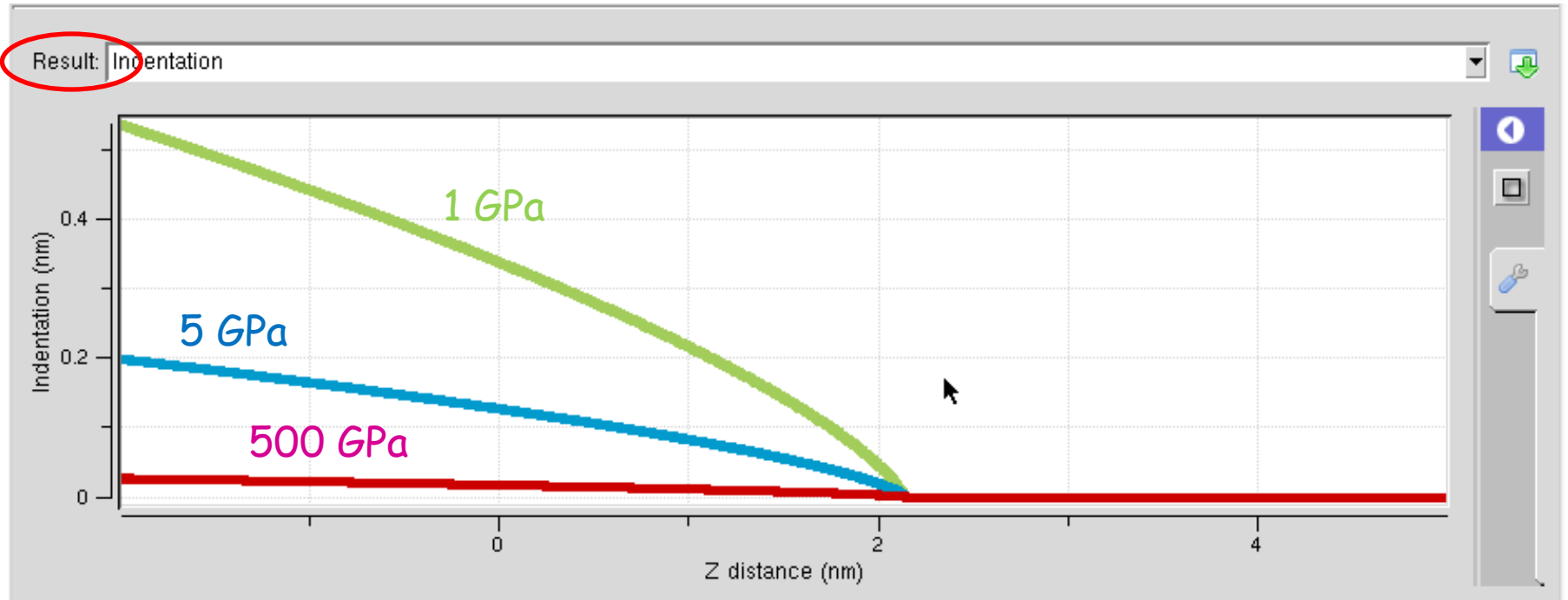


-2 nm

Remember: $d = z + q$

+5 nm

Indentation vs z (vary E_{sample})



Up Next: Contact Mode Scanning