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

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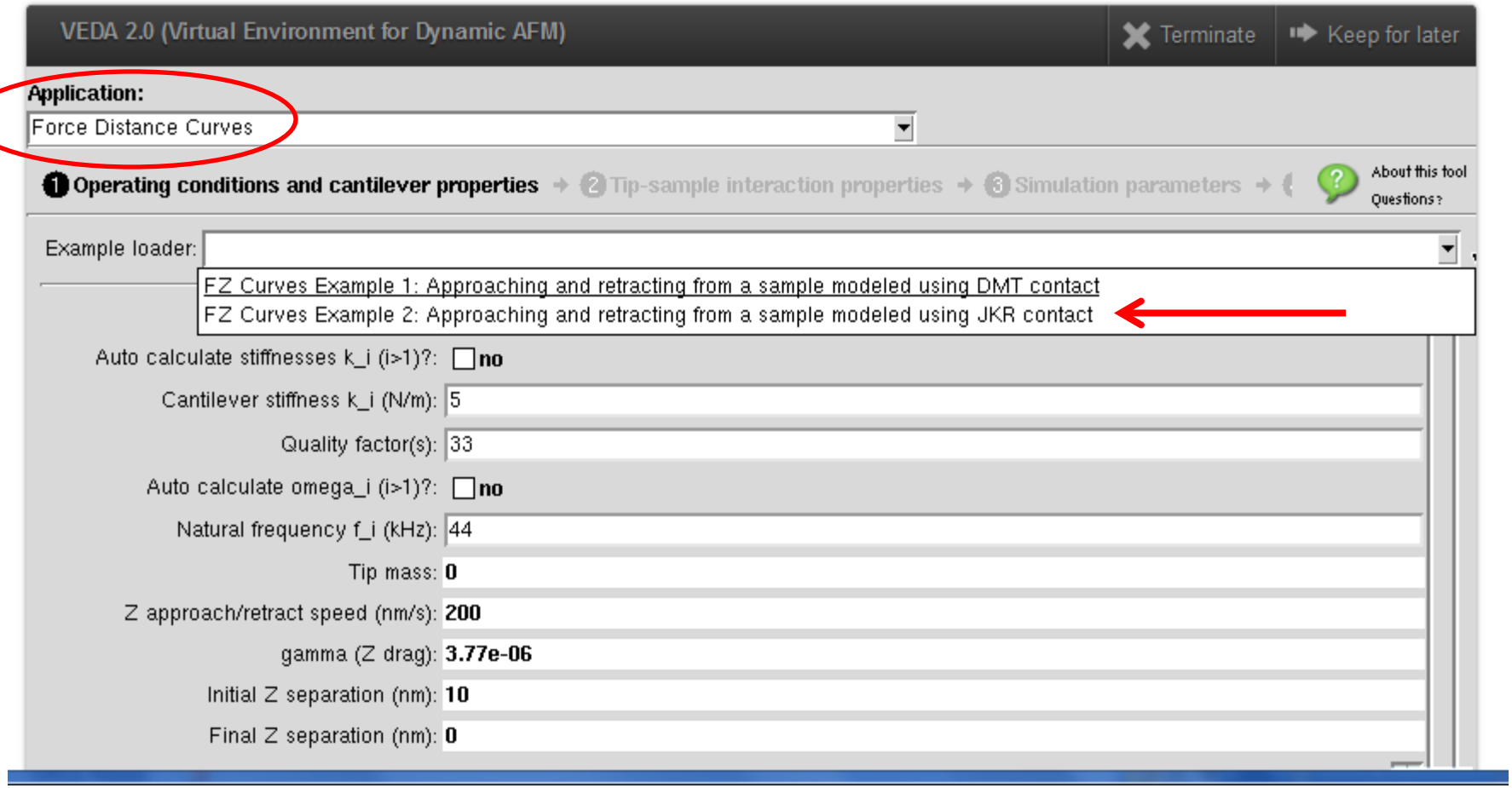
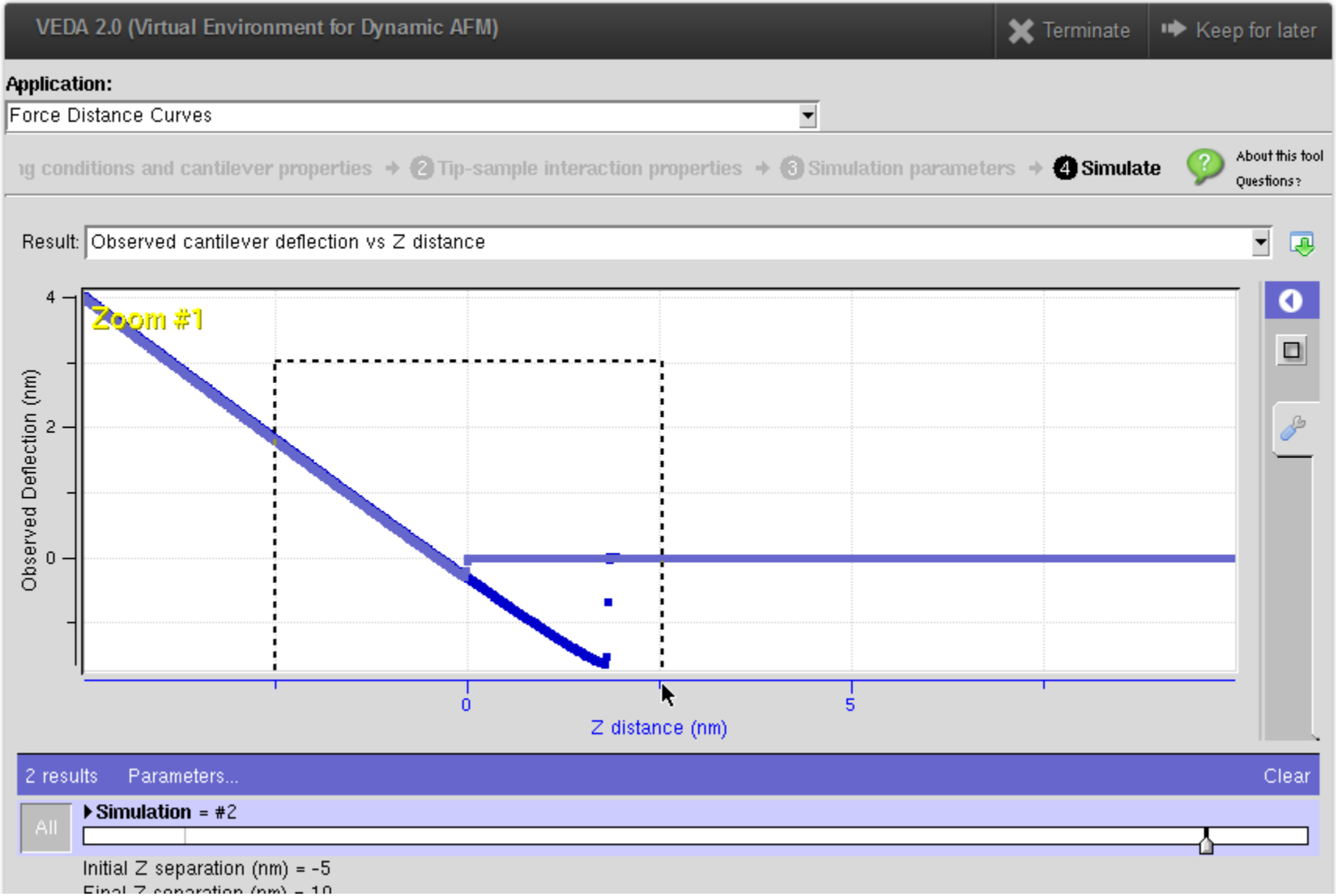
VEDA has a number of examples preloaded



JKR approach and retract curves

k_{tip}=0.87 N/m R_{tip}=10 nm E_{sample}=1 GPa

Zoom in on features of interest



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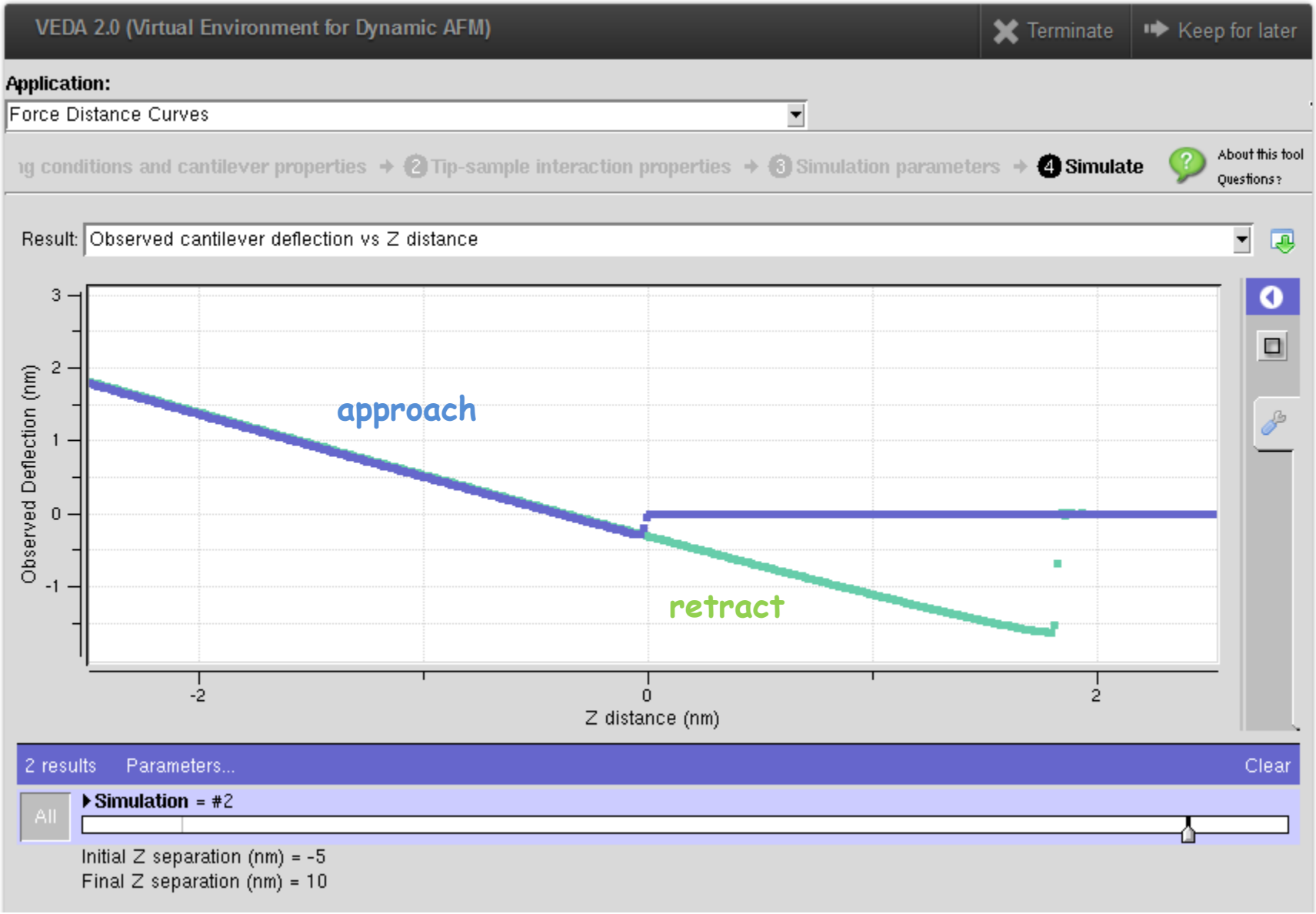
Plot after enlarging



P1_Wk5_L2

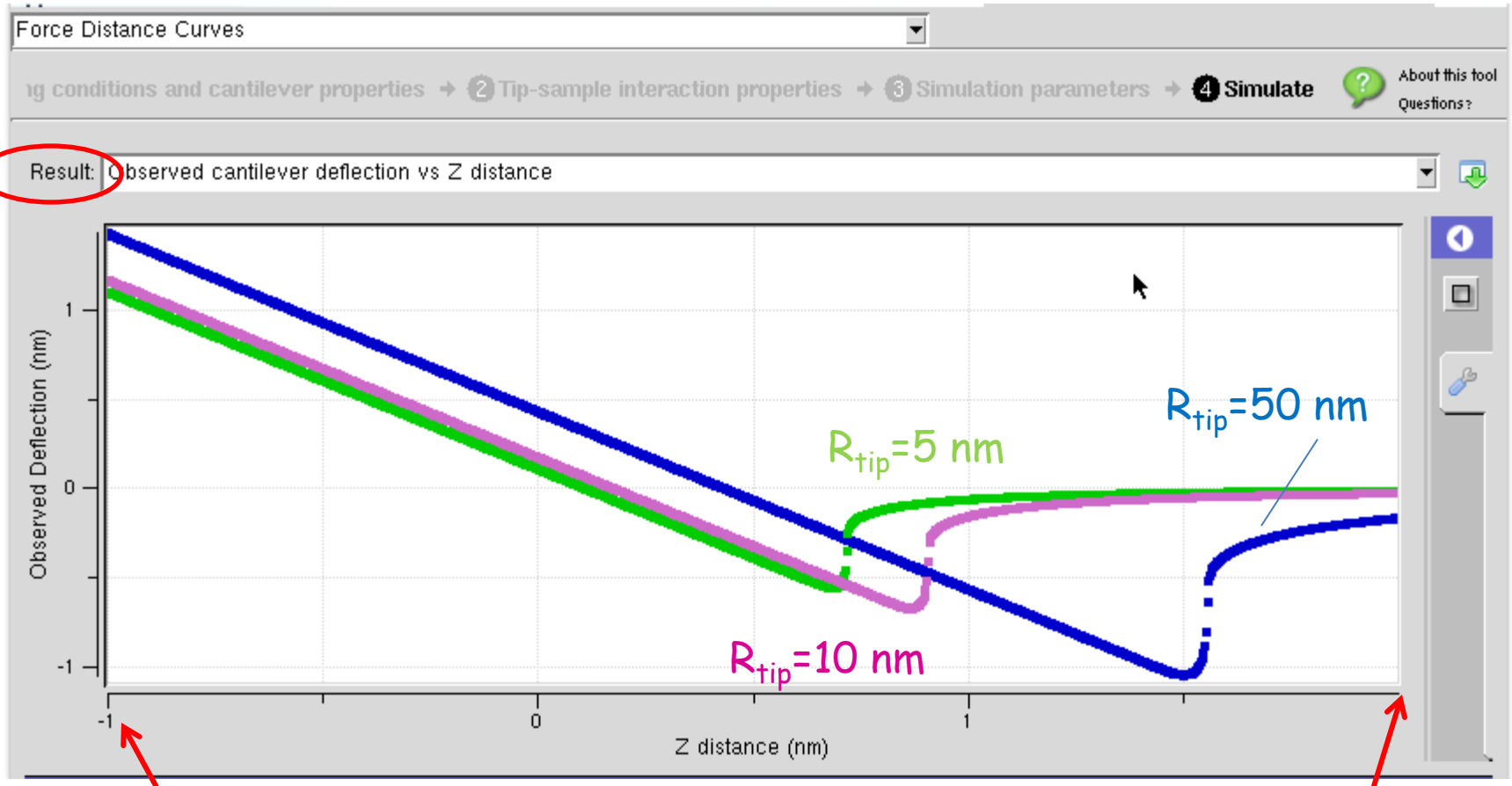
Example 1:

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_{tip} = 5 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

P1_Wk5_L2

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.

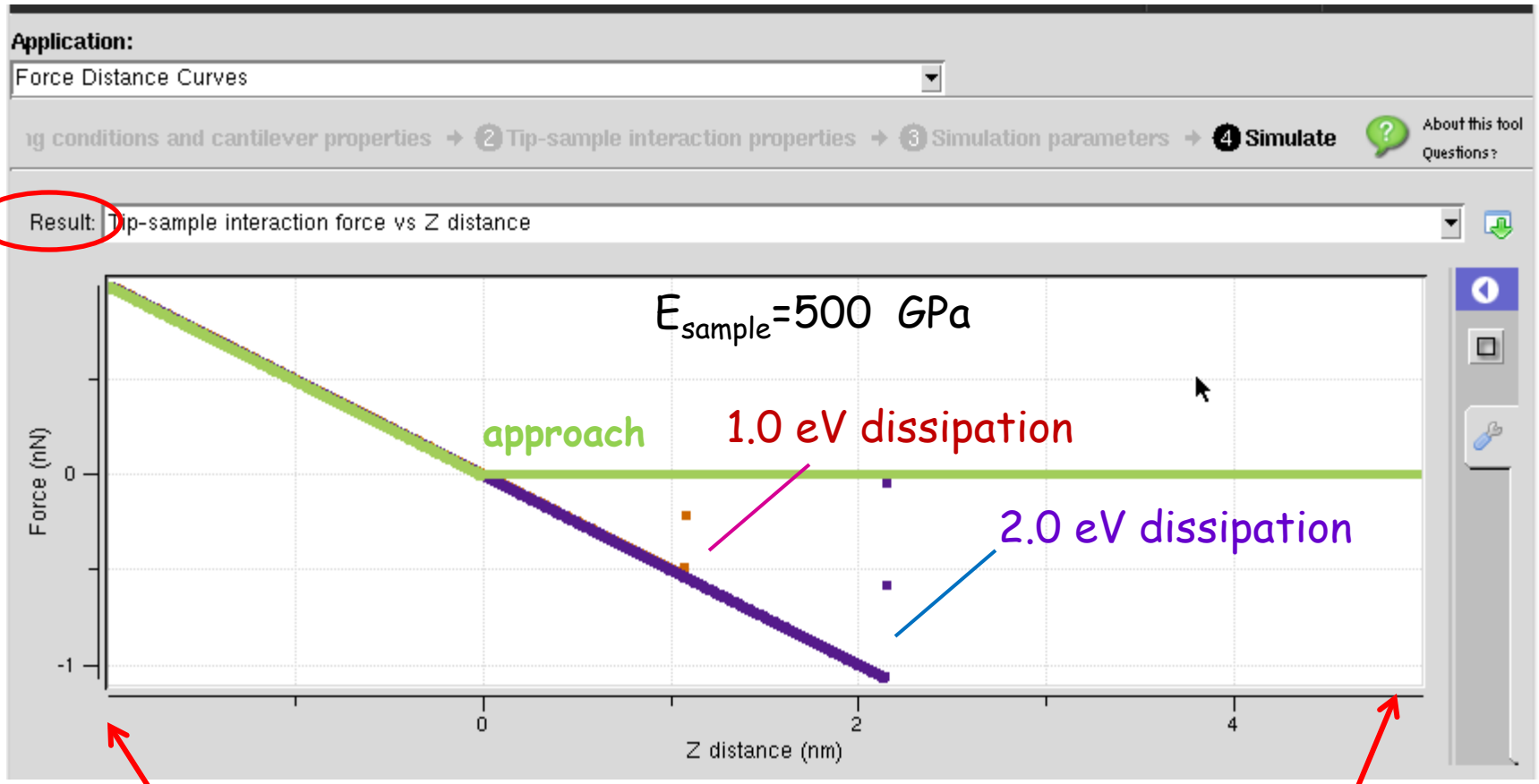
Use the default values provided by VEDA for other parameters.

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) 0.000000000000000E+000
LockInOrder 0
mtip 0
omegad 44
Ainitial = 1
AprchS 200
gamma_drag 3.77e-06
omega = 44
Keq = .5 k_{cant} = 5 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 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 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 5
-2 nm < z < +5 nm
plotpnts 1000 numincycle 1000
transient_allowance

Capillary adhesion

Force vs. z



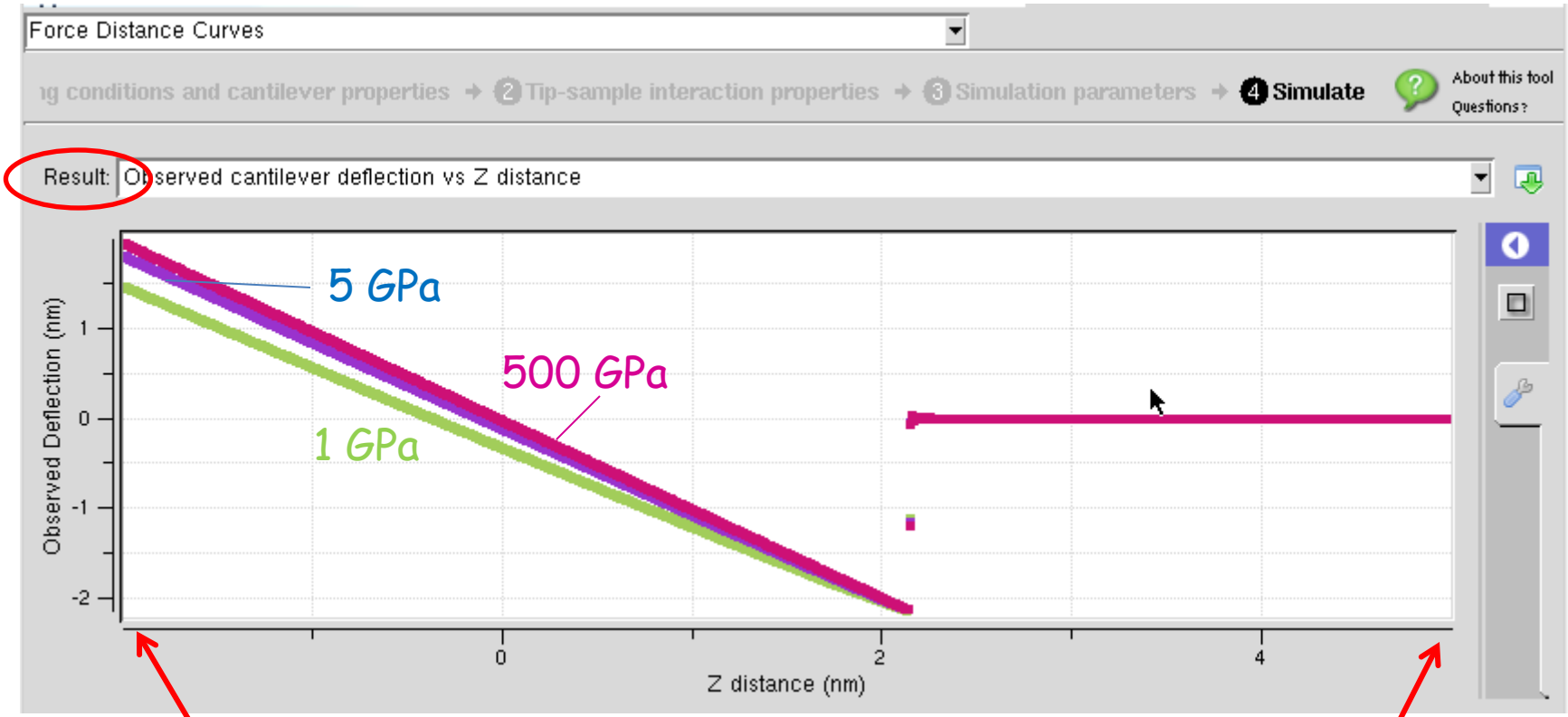
-2 nm

+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

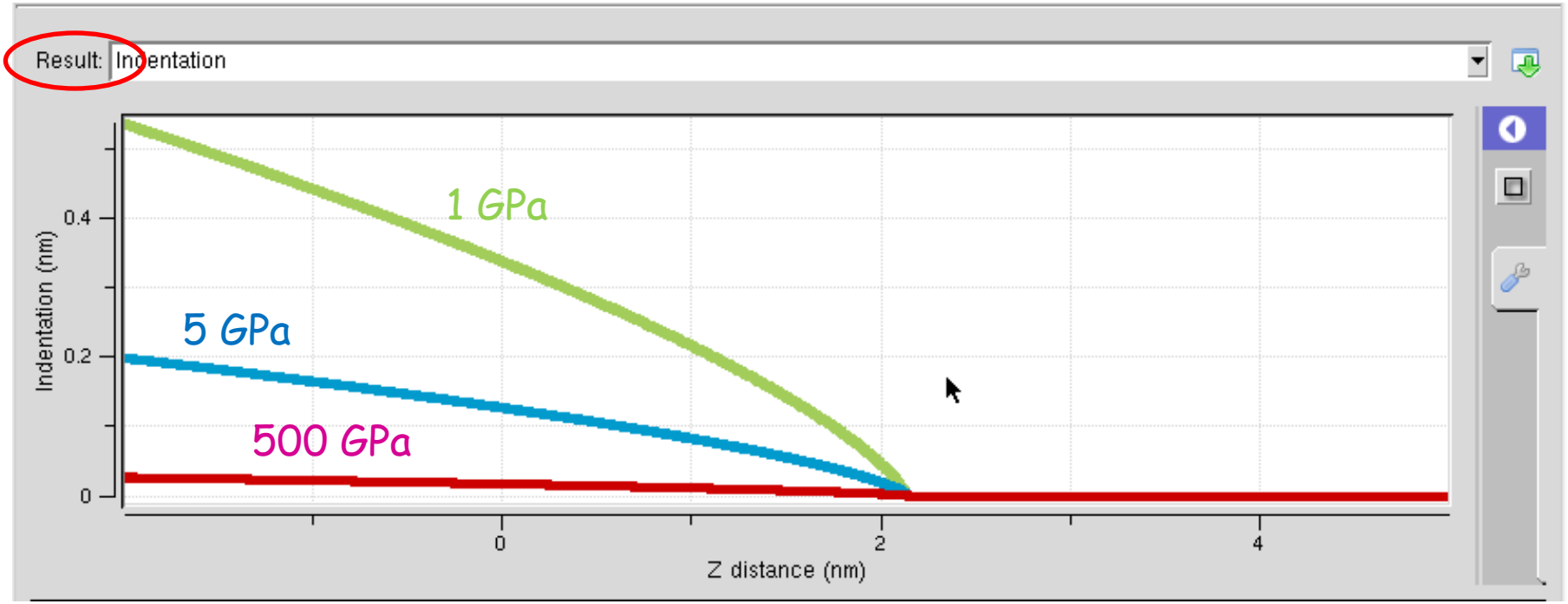


-2 nm

Remember: d=z + q

+5 nm

Indentation vs z
(vary E_{sample})



Up Next: Contact Mode Scanning