

# Lecture: P1\_Wk5\_L3

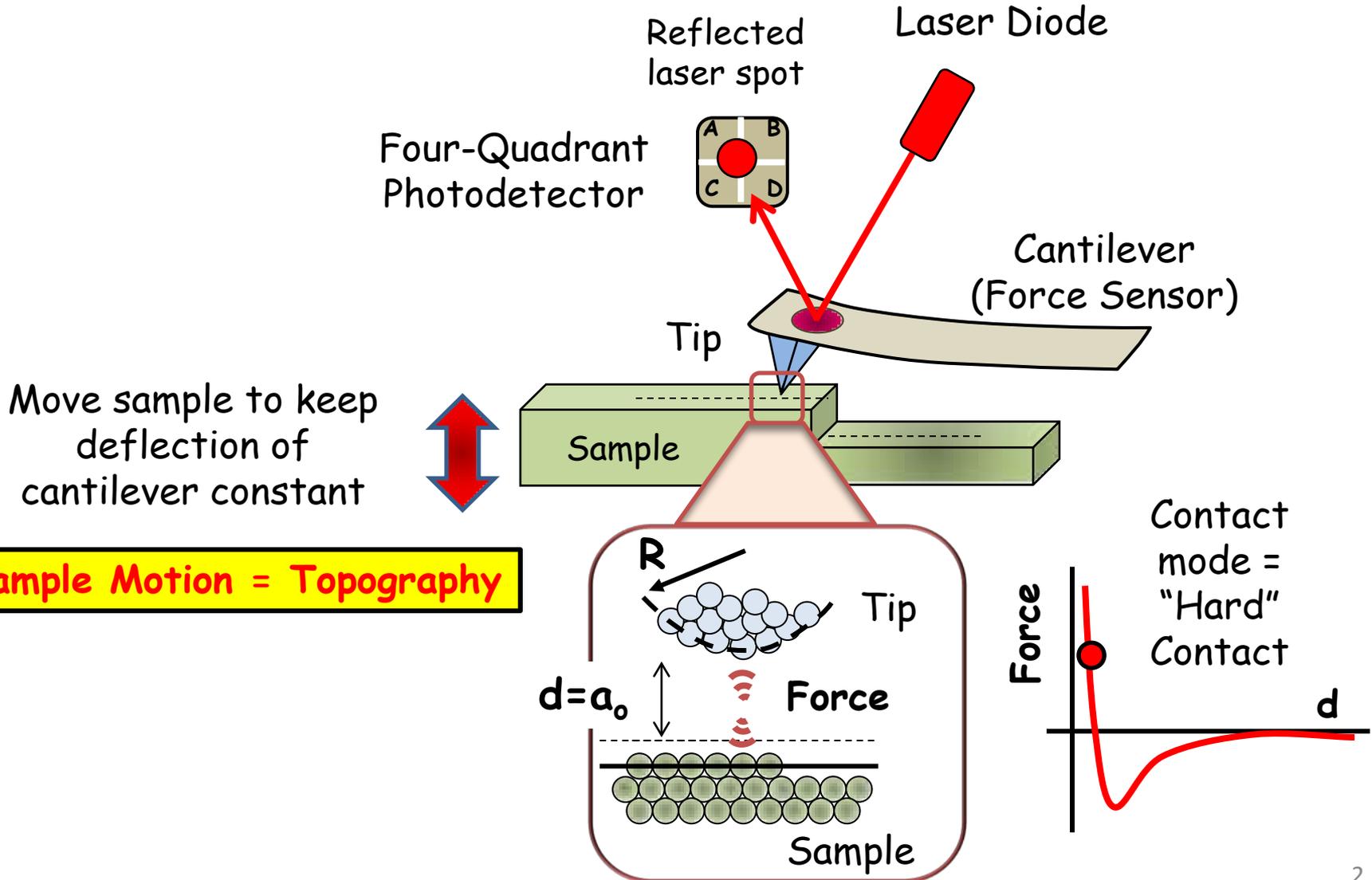
## Contact Mode Scanning Simulations with VEDA

Ron Reifenberger  
Birck Nanotechnology Center  
Purdue University  
2012

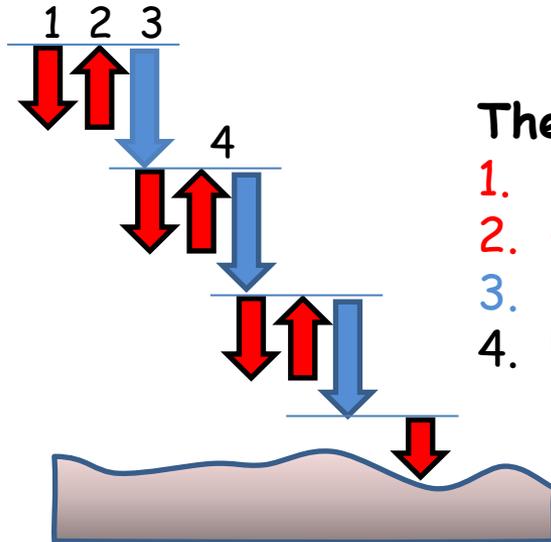
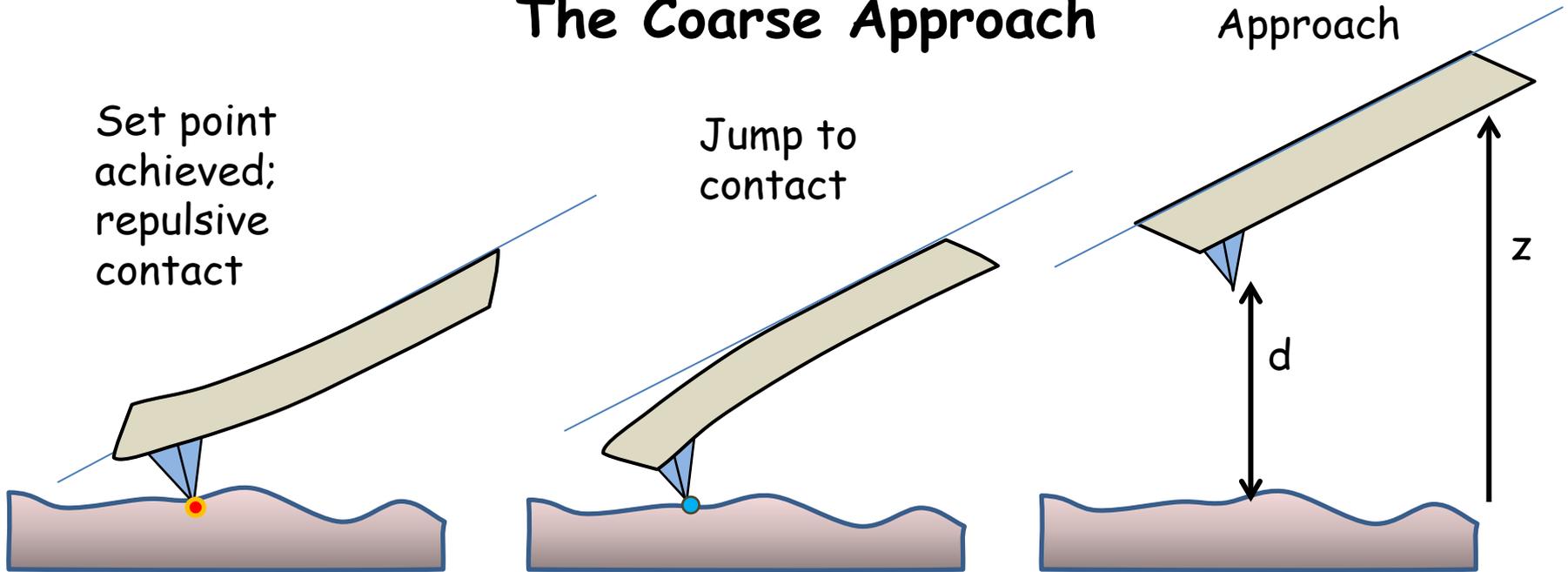
for VEDA overview: Rev. Sci. Instrum. 83, 013702 (2012).

# The Purpose of a Microscope is to Obtain an Image

See P1\_Wk3\_L5



# The Coarse Approach

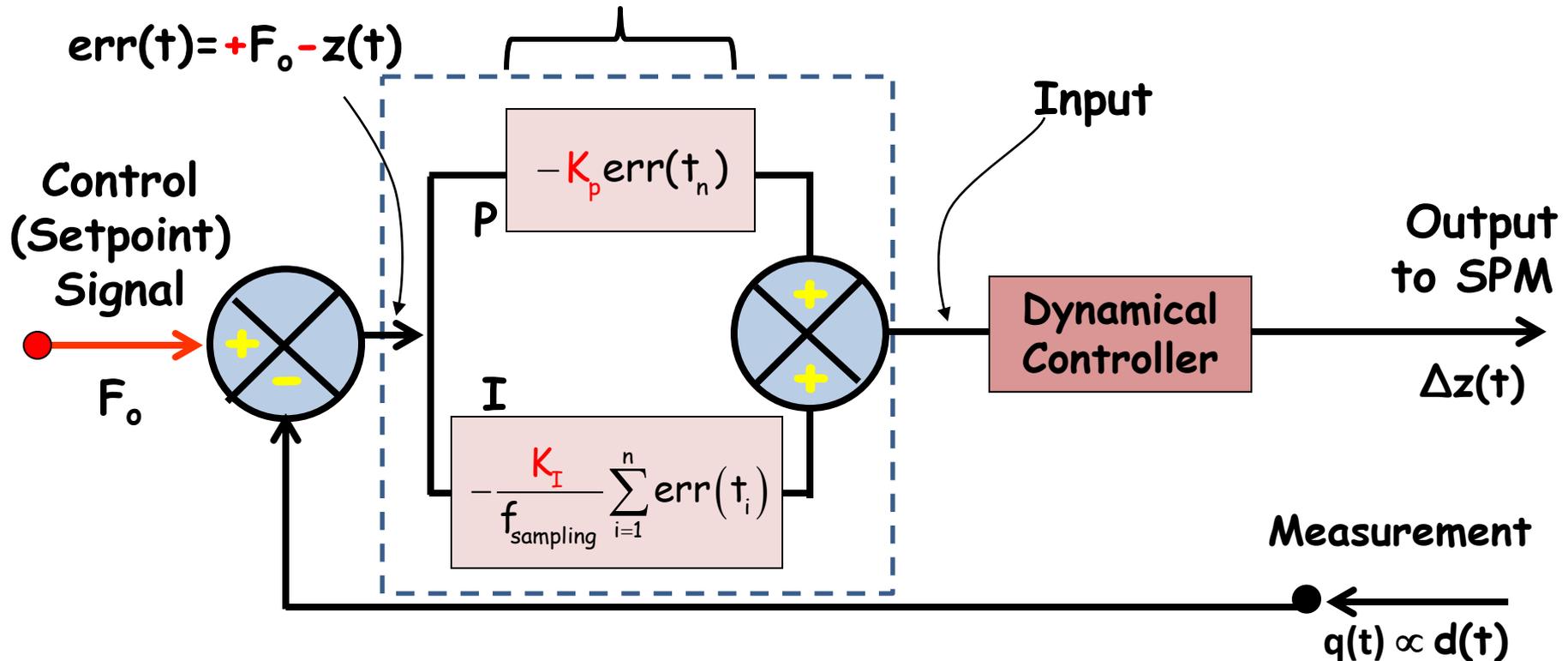


## The coarse approach sequence:

1. **Slowly** expand z-piezo
2. **Quickly** retract z-piezo
3. **Stepper motor advance**
4. Repeat until force setpoint is reached

# The AFM Feedback Loop

## Control Law



- The proportional (P) controller allows the probe to follow smaller, high frequency features by adjusting  $K_p$
- The backward integrator (I) controller allows the probe to follow larger, low frequency features by adjusting  $K_I$
- $f_{\text{sampling}}$  should be  $\sim 10x$  the frequency of the most relevant feature that is being measured

# Contact Mode Scanning in VEDA

Go to the NanoHub at <http://nanohub.org/> and login to your account.

Locate the VEDA software and launch the tool.

Select the "Contact Mode Scanning" application.

For this application, there are five key "tabs" labeled:

- ① Operating cond. + Cantilever prop.
- ② Tip-sample interact. Prop: substrate
- ③ Simulation parameters
- ④ Tip-sample interact. Prop: Feature
- ⑤ Simulate

# Under

## ④ Tip-sample interact. Prop: Feature Select "Step"

VEDA: Virtual Environment for Dynamic AFM (11:58 pm) [X] Terminate [▶] Keep for later [Block...]

**Application:**  
Contact Mode Scanning

Tip-sample interact. prop: substrate → ③ Simulation parameters → ④ Tip-sample interact. prop.: Feature → ⑤ Simulate [?] About this tool Questions?

Select a geometric feature: Sinusoid

Feature height (nm): 30

Length of feature (nm): 50

Length of trapezoid top (nm): 30

Include geometric convolution:  no

Specify material properties:  no

To specify separate properties for the feature, select "yes."  
Click to turn on/off

**Step**  
Trapezoid  
Sinusoid  
Cylinder

## Example 1:

Perform a contact mode scanning simulation on a sample that has a step of height 10 nm and a length of 50 nm.

- a) Under the **Operating conditions** tab, set the following parameters to specify the cantilever and the controller properties:
  - One eigenmode for the cantilever,
  - Cantilever stiffness of 3 N/m,
  - Quality factor of 100,
  - Natural cantilever frequency of 40 kHz,
  - Setpoint deflection of 4nm,
  - Scan lines/second = 10,
  - Proportional and integral gains of 0.005.
- b) Under the **Tip-sample interaction properties: substrate** tab, choose the DMT contact (with all its default values) to specify the tip-sample interaction.
- c) Under the **Simulation parameters** tab, set the scan size to 100 nm.

Run a simulation. What do you observe in the measured topography when

- the tip approaches the feature
- the tip moves past the feature

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

```

exc_choice = 1
operating mode 3 fexcite 3 numModes
1
LockInTC (us) 0.0000000000000000E+000
LockInOrder 0
mtip 0
omegad 9.3
Ainitial = 1
omega = 40
Keq = 3.0
Chi = autocalc
Q = 100
sample_freq Mhz 1
sample_freq 1000000.00000000
LineSpeed 10
SNratio 60
KP 0.005
KI 0.005
HF 10
LF 50
LF2 30
LS 100
Feature type
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

```

$k_{cant} = 3 \text{ N/m}$

Scanning speed

P, I feedback gains

10 nm high step that is 50 nm wide

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

Indicates that  
 tip-sample convolution  
 is turned off. This is  
 the default - it makes  
 the calculation easier.  
 BEWARE: the  
 topography plotted is  
 for a tip radius of zero.

```

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
Example 1
Poisson_sample 0.3
KD 0.001
epsilon 80
sigmat -0.0025
sigmas -0.032
hs 6
want presiach F
Zrange 0
plotpnts 1000 numincycle 1000
Asp 4
transient_allowance

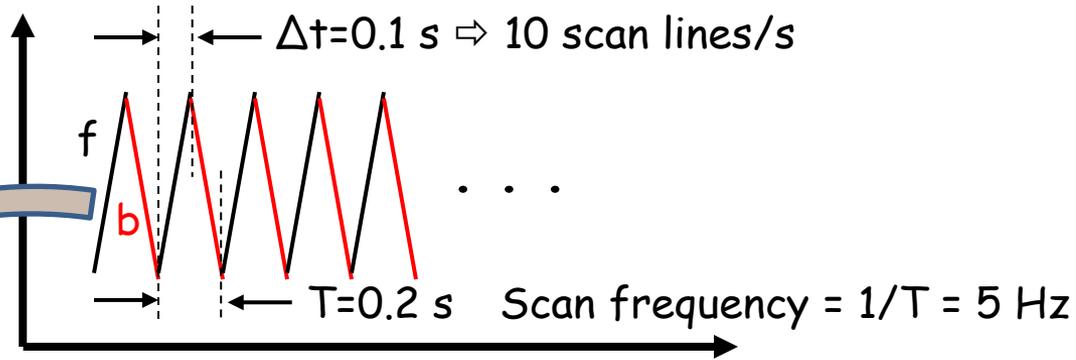
```

Modulus of sample = 1 GPa

# Tip Speed

When you choose 10 scan lines/s, you are specifying the tip velocity as well as the input signal to the x-piezo

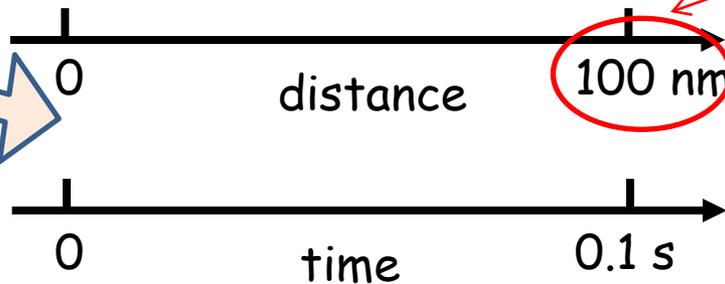
Signal to x-piezo (in Volts)



$f$  = forward scan

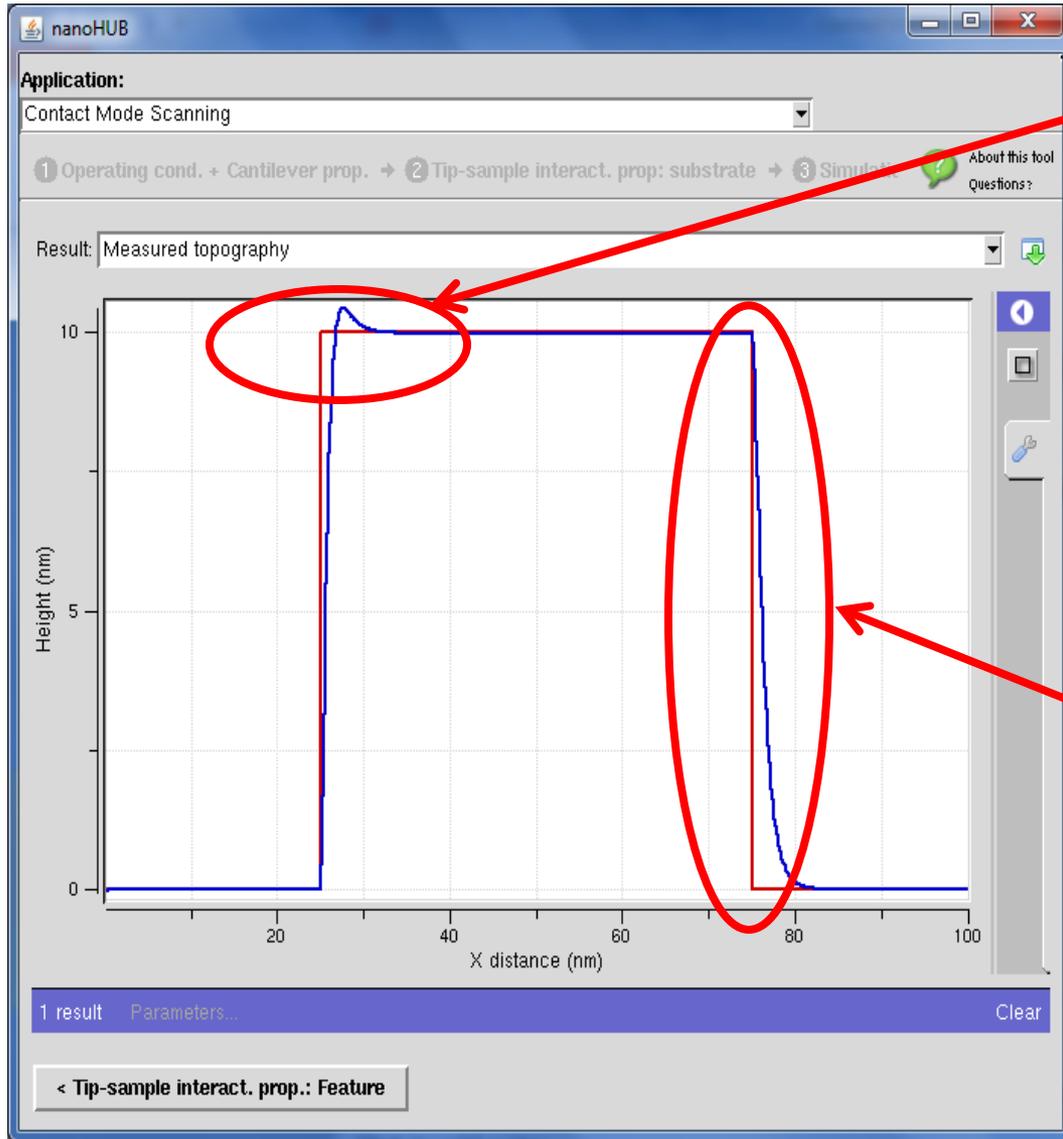
time

Specified under the "Simulation parameters" tab



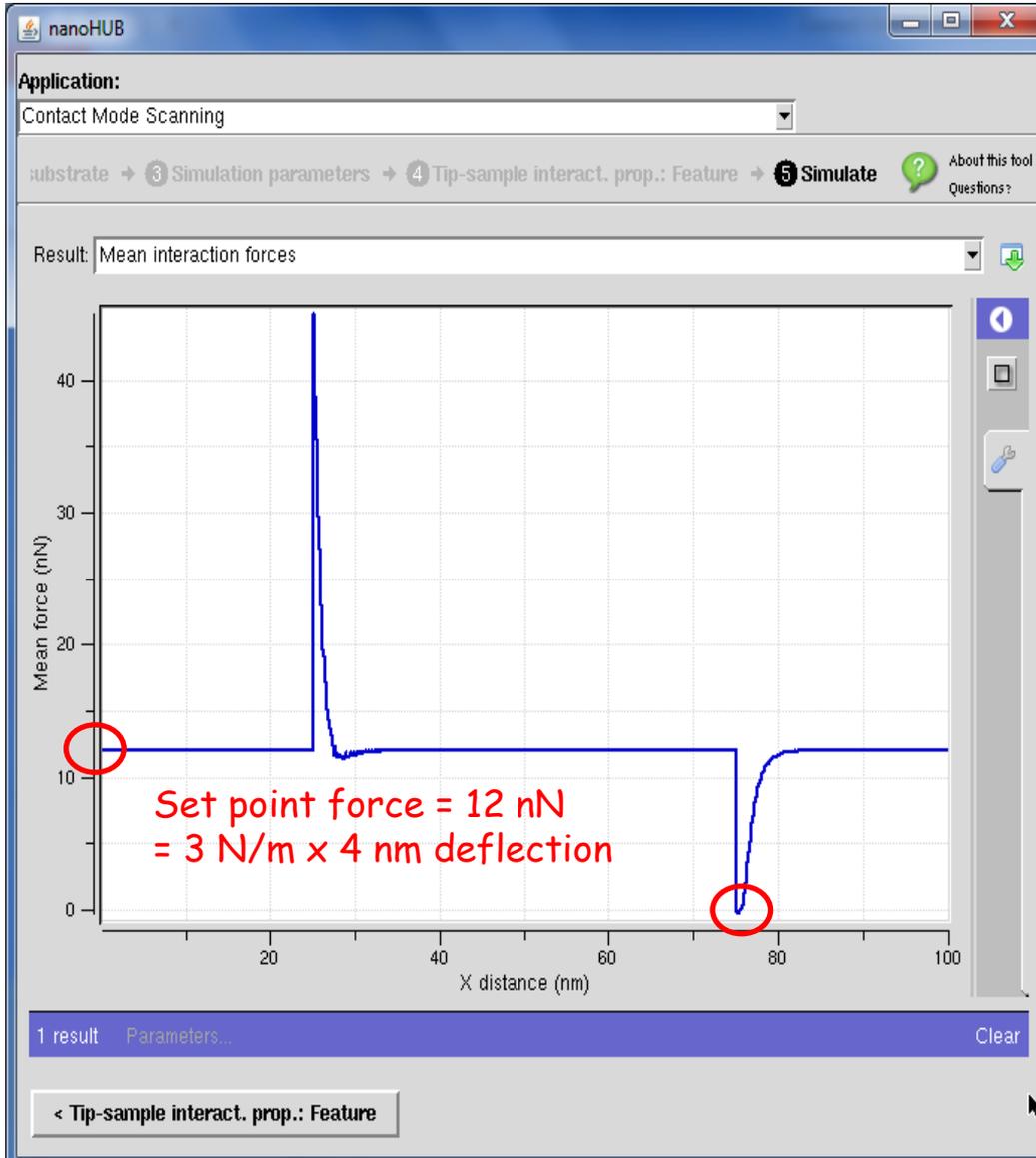
$$v_{\text{tip}} = \frac{100 \text{ nm}}{0.1 \text{ s}} = 1 \text{ } \mu\text{m/s}$$

# Result of Simulation



- The red curve is a plot of the geometric feature.
- The blue curve is a plot of the **z-piezo response** assuming **zero tip radius**. The z-piezo response **approximates** a topographic map of the sample.
- Depending on P&I, there is a finite time required for the controller to react to the step height.
- As plotted by the blue line, the controller changes the z-distance to maintain the specified setpoint deflection.
- When the tip moves past the feature, the cantilever deflection suddenly decreases as the tip is no longer in contact.
- The controller now readjusts the z-distance until the tip finally comes in contact with the sample and reaches the set point force that you specify<sup>10</sup>.

# Mean Interaction Force

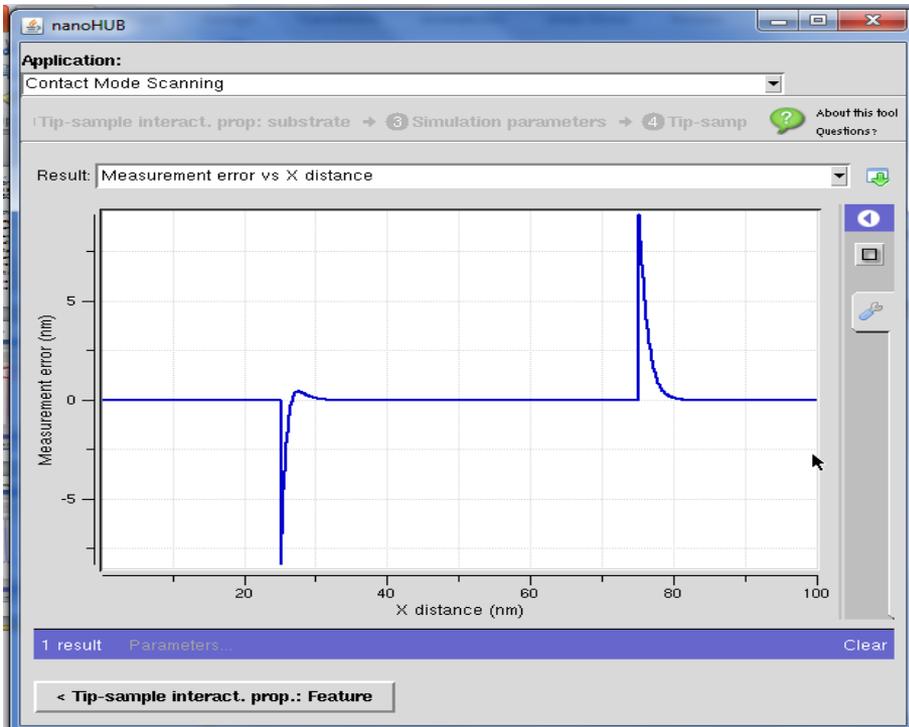


When the feature is encountered the mean force quickly rises.

Once the controller recognizes the feature, the z-distance is altered to keep the deflection (and hence the force) constant. The controller is not perfect, so there is a momentary increase in the mean interaction force.

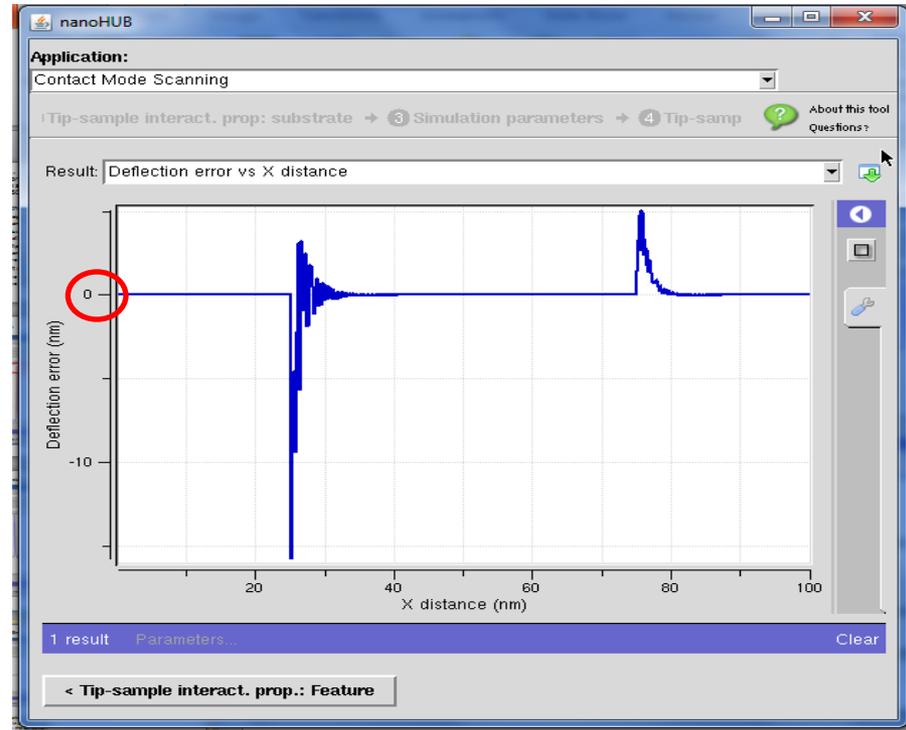
When the tip moves past the feature, the cantilever is no longer in contact with the sample and hence the mean force momentarily goes to zero until the controller regains the set point.

# Measurement Error:



This graph shows the difference between the actual topography and that measured by the AFM.

# Deflection Error:



The feedback control parameter in contact mode scanning is the deflection.

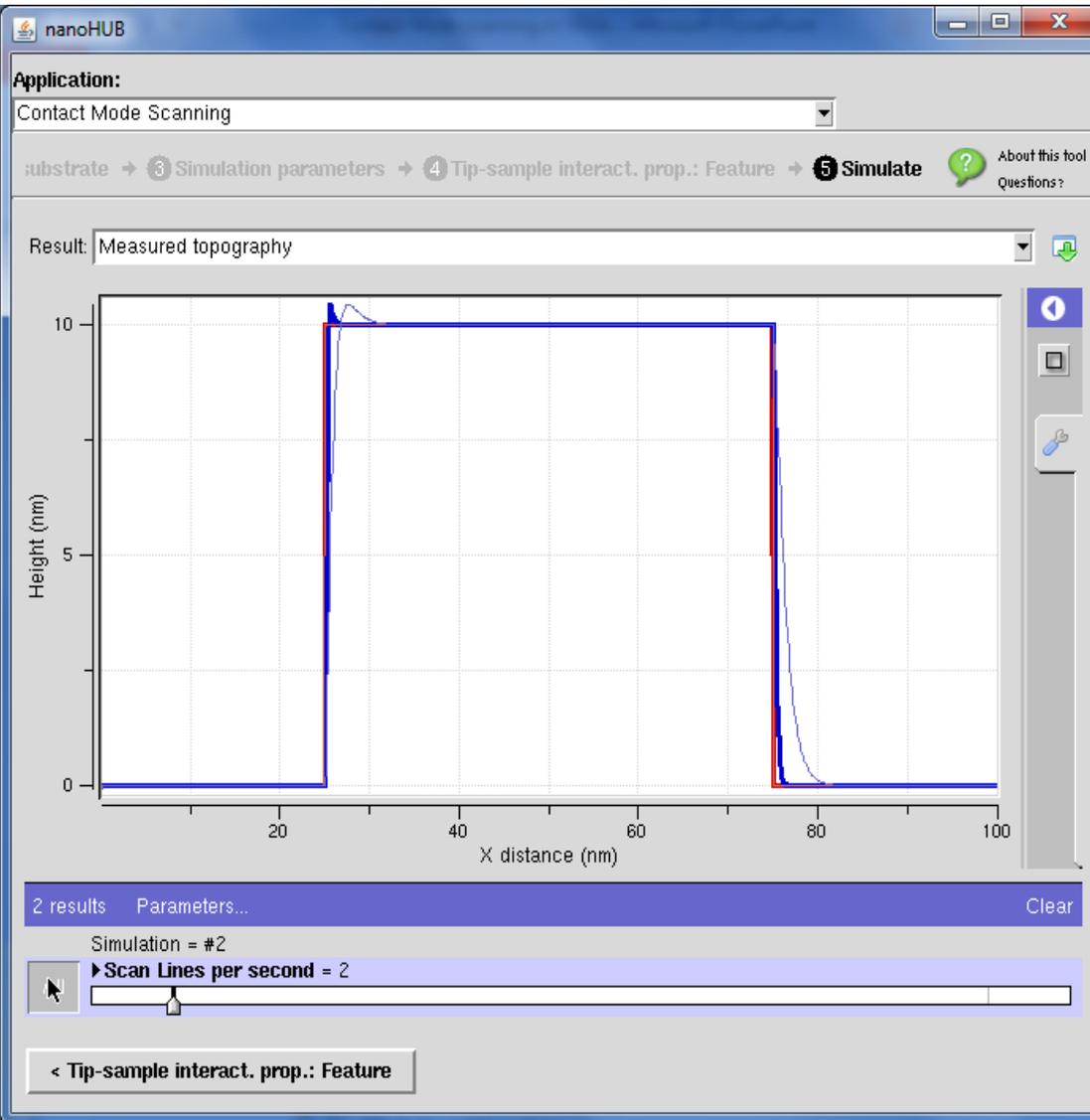
This graph shows the **difference** between the cantilever deflection while scanning and the setpoint deflection (which was specified as 4 nm) when setting up the simulation.

Can we do better? Reduce the scan lines per second to 2 lines/sec and look at the change in the measured topography.

You should get:

By reducing the tip scan velocity, the controller has more time to respond to changes in topography.

Note: the feedback gain values can also be adjusted to reduce the effect of parachuting. This will be discussed in the upcoming lectures.



# What if you include the finite radius of the tip?

**Application:**  
Contact Mode Scanning

1 Tip-sample interact. prop: substrate → 3 Simulation parameters → 4 Tip-sample interact. prop.: Feature → 5 Simulate  About this tool  
Questions?

Select a geometric feature: Step

Feature height (nm): 10

Length of feature (nm): 50

Length of trapezoid top (nm): 30

Include geometric convolution:  yes

Specify material properties:  no

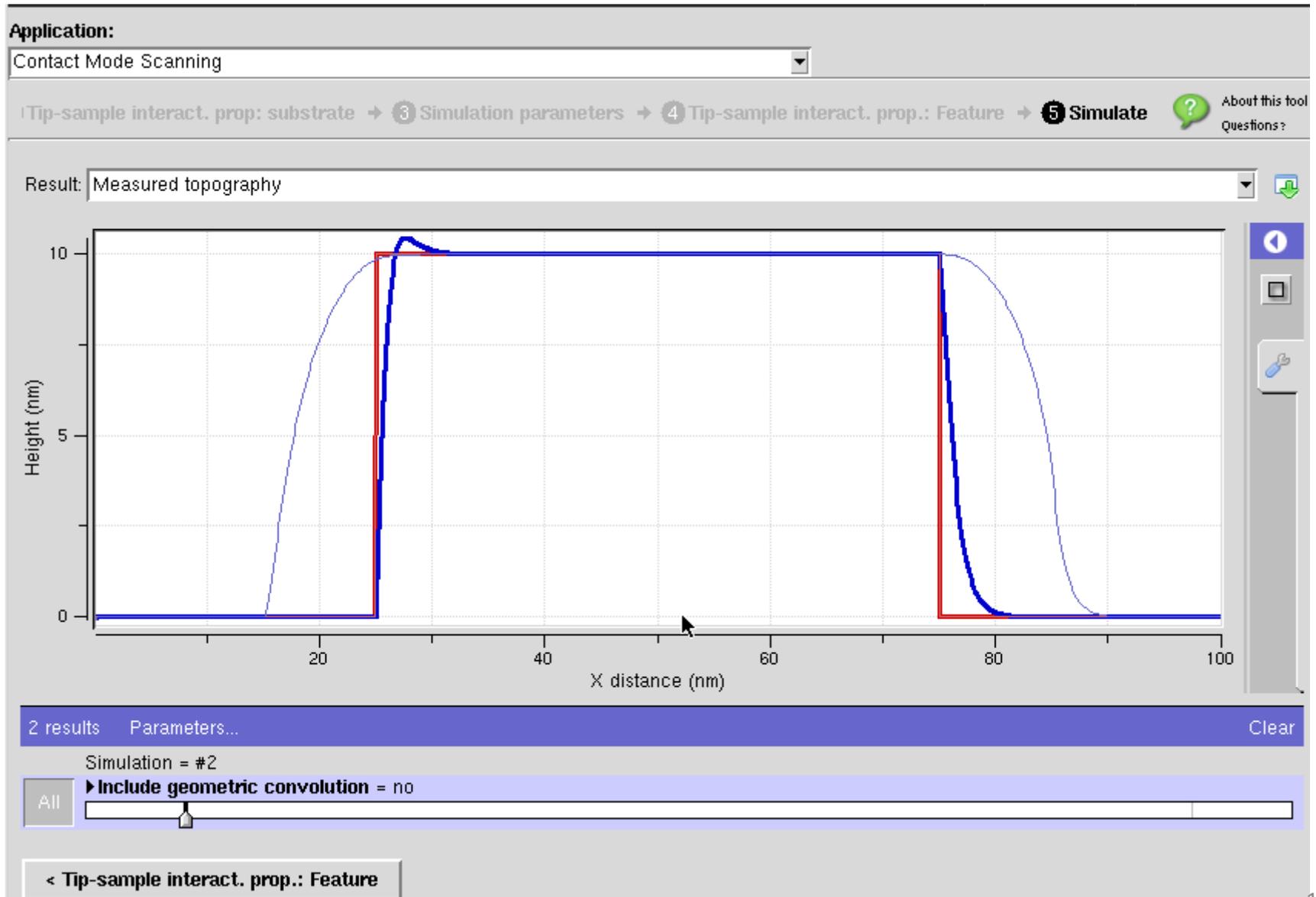
*Click the geometric convolution box until it says :yes"*

**Notes:**

1. The time required for the simulation now increases. It may take a minute or more to complete the simulation.
2. If the feedback parameters are not properly set, the initial setpoint will not be achieved and the simulation will "time out" just searching for the set point. Readjust the P and I feedback gains..

< Simulation parameters Simulate >

# Results of tip convolution on topography



**Up Next: More Contact Mode Scanning Examples**