

Optical Tweezers

Draft Design
Jan 29, 2007

Changes

- Make light grey box frame around laser control panel that matches handles.
- Make grey supports looking like they are supporting the lens.
- Make control panel section that's title "Graphs" with radio buttons for None, Position Histogram, and Potential Energy Curve
- Make control panel section that's titled "Laser Display" as radio buttons
 - Beam
 - Electric field vectors
 - Beam with vectors

Behavior would be that Beam was only option in fast mode, but other radio buttons became active in super-duper slow mode.
- Make control panel section that's titled "Bead's charges" as radio buttons
 - Hidden
 - Charge distribution
 - Excess charge only
- Rail-slider for laser
- Make lens with flat view

Changes meeting – w/ Wendy : June 4, 2007

- Reduce spacing between radio buttons
- Add “Ignore brownian motion” option, delete “show brownian force”
- Add ruler icon next to show ruler

Concepts

- Concepts for 1st panel: Physics of Tweezers
 - Light is oscillating, propagating electric field
 - Electric field induces a polarization of the bead. This polarization increases with strength of electric field, and changes direction with change in direction of E-field
 - Gradient in electric field and polarization of bead causes net force towards center (**show force in x only???**)
 - Show as balance of right hand side force and left hand side force
 - Bead is under constant brownian motion
 - Distance that bead travels is balance of brownian motion versus trap strength: $\frac{1}{2} k_B T = \frac{1}{2} k_{x\text{-trap}} \langle x^2 \rangle$
 - If bead is out of trap it will just undergo brownian motion.
 - ON FREEZE FIELDS OR PAUSE view, learning goal:
 - Moving bead around changes polarization of charges and net force on bead.
 - (DON'T DO THIS?) Allows you to let go and see behavior of bead in a “static” E-field
 - How to model this???
 - Static field you won't get k-trap ... take example of when you are at zero e-field (no force).
 - (DO THIS) Possibly just allow them to move bead around during “PAUSE” (showing force vector) but not model motion of ball with static E-fields.

- Start-up ideas:
 - No bead?
 - Or bead out of beam ... with wiggle me of move bead into laser?
 - Or bead doing brownian motion with no laser on and wiggle me to turn laser on?

Physics NOT shown...

- Right now cannot change radius of bead (could add to advanced features if important).

Physics of Tweezers

User Stories:

1) Trap force like a spring:

- a. User grabs bead and moves it horizontally. Sees force grow as distance from center grows. Always towards center
- b. User goes to advanced options and sets flow going. Calculates offset of bead in x versus flow force ... $6 \pi \eta r v = k_{\text{trap}_x} X$. (They will have to estimate r of bead with ruler, viscosity and velocity are from controls.)
- c. Intensity control changes force.

2) Can control position of bead with laser:

- a. User grabs laser and drags it around seeing that bead will stay in laser beam unless user moves laser “stage” too fast. In which case bead will “pop” out of laser beam and just be doing brownian motion.
- b. Intensity control changes speed at which bead pops out.

3) ETC... I can write a ton, but before I do I want to make sure this is what Chris wants.

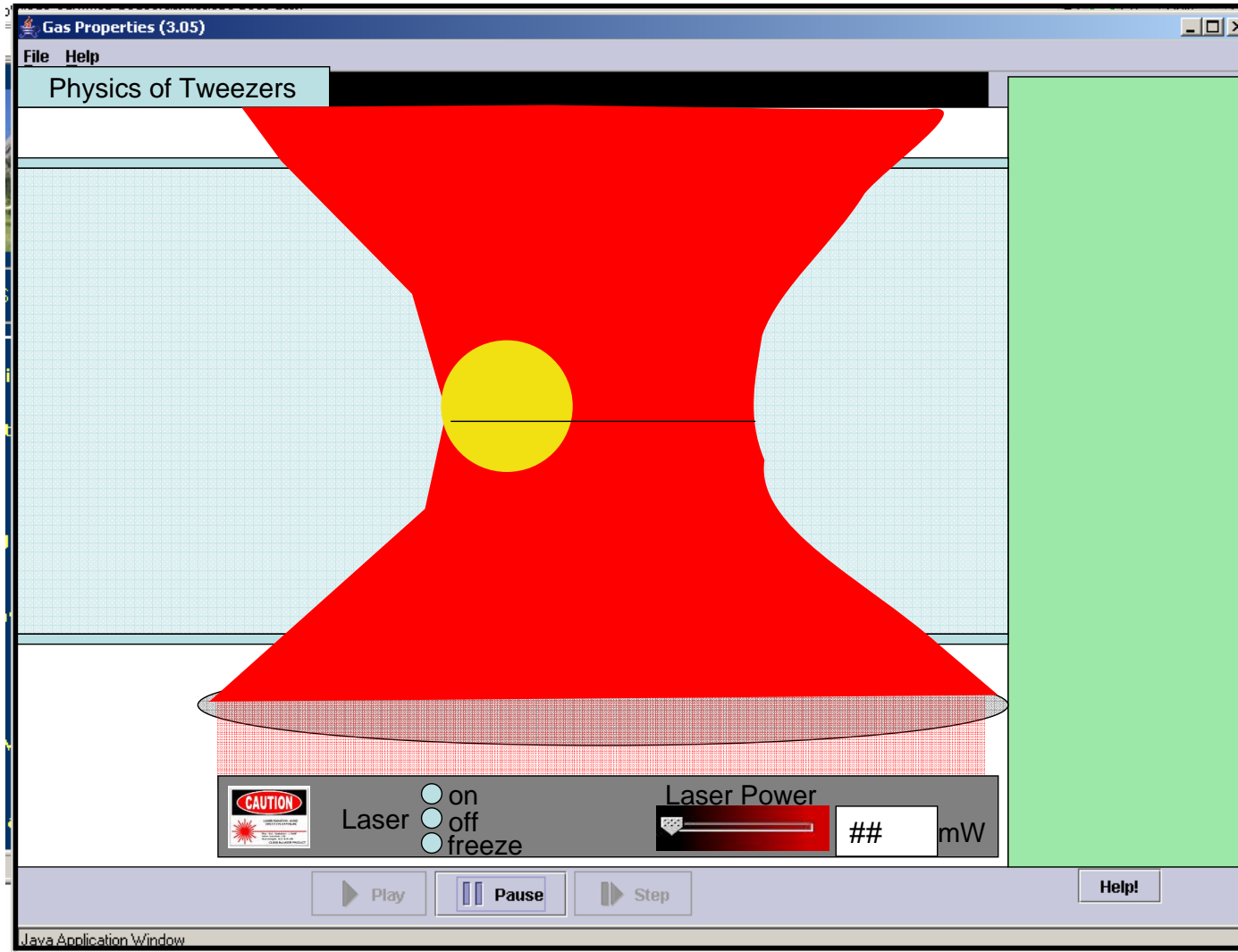
Physics of Tweezers

Dimensions:

- Bead is 200nm
- Laser waist is 500 nm

Look:

- Bead should have shading to look 3D
 - Laser should have shading so that red looks like gaussian power distribution from left to right and weaker where broader beam.
- Red should get brighter with intensity.

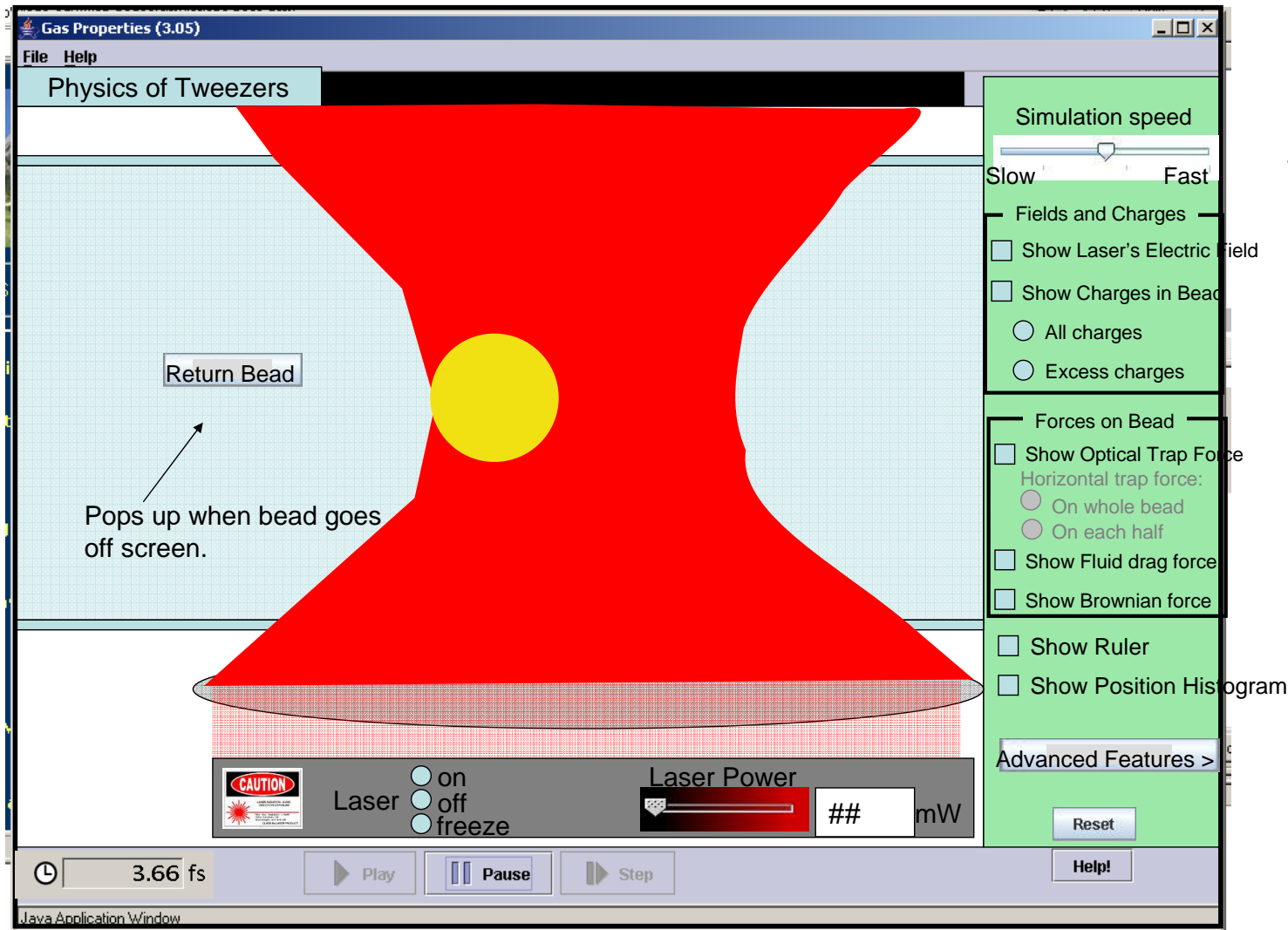
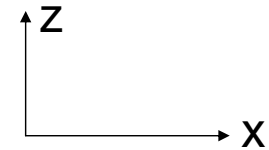


Basic idea:

- Bead in liquid undergoes brownian motion
- Laser beam ON puts force on bead that pulls it toward center of laser beam .. “traps it”
- Liquid is viscous so causes bead to always moves at terminal velocity (Force ~ velocity NOT Force ~ acceleration).

Physics of Tweezers

Sim speed = FAST (Shows only time averaged forces on bead)



Laser force is like a SPRING force:

$$F_{\text{trap}_x} = k_{\text{trap}_x} \cdot \Delta x$$

$$F_{\text{trap}_z} = k_{\text{trap}_z} \cdot \Delta z$$

Δx = distance from center in x

Δz = distance from center in z

Trap force goes to zero if bead is

Force on bead given by k_{trap} :

$$k_{\text{trap}_x} = \text{Power} / 11400$$

Power in mW, k_{trap_x} in pN/nm

k_{trap_x} is independent of z.

Power goes from 0 mW to 1000 mW

$$k_{\text{trap}_z} = k_{\text{trap}_x} / 5.6$$

$$F_{\text{drag}} = \gamma \cdot \text{velocity}$$

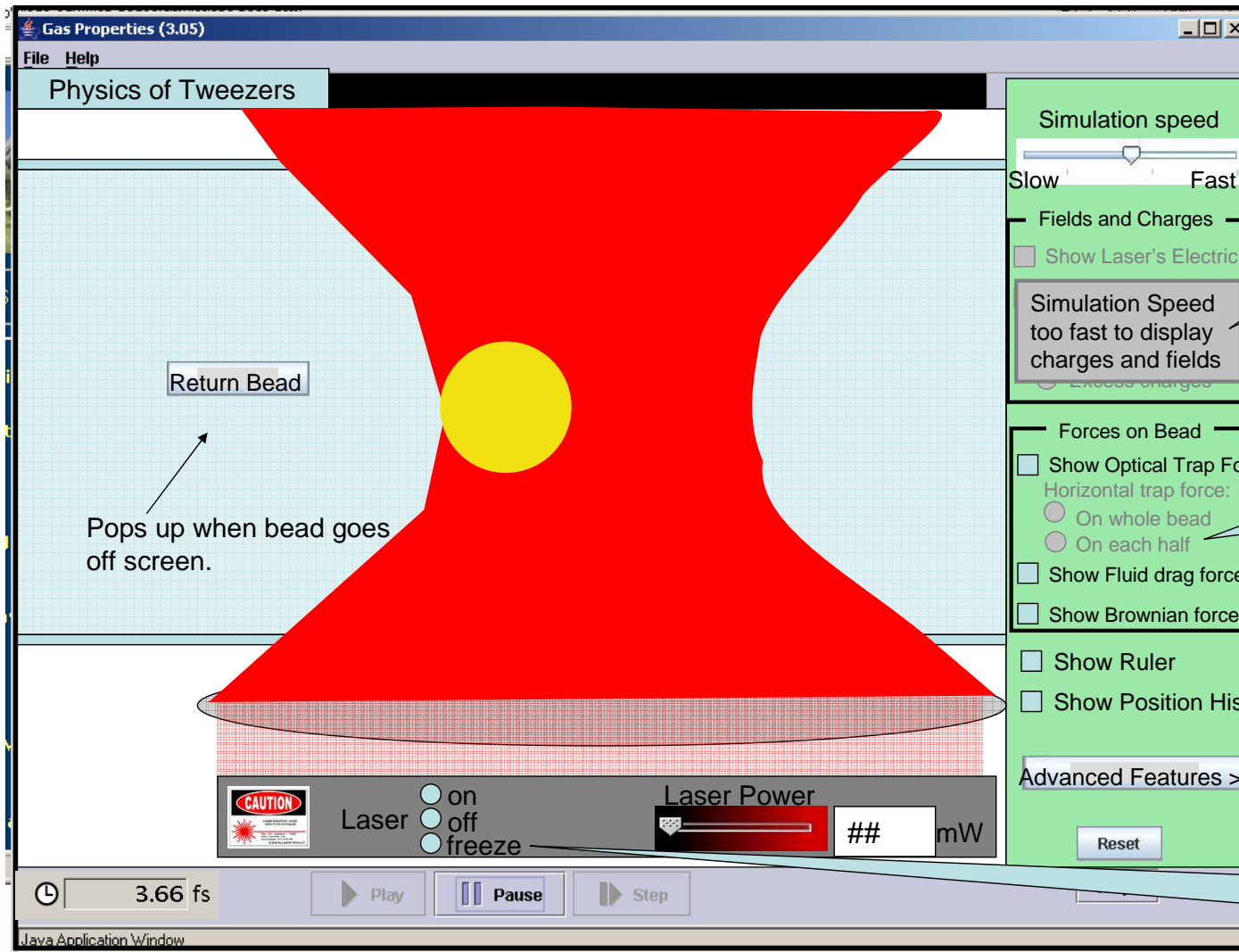
(γ = drag coefficient, will be adjustable through viscosity in advanced features)

F_{brownian} = small random kicks

Model check: If No force ... (laser off)
diffuses ~1 bead diameter in 1 sec

Physics of Tweezers

Sim speed = FAST (Shows only time averaged forces on bead)



If sim speed is fast, have message appear in this part of control panel that says cannot display this now.

Grey out this control if sim speed too fast to display fields and charges.

Is it reasonable to display Brownian motion forces?? Need to check modeling.

May want "laser freeze" or just use "pause" button if can allow dragging bead around if that is active?

Physics of Tweezers

Sim speed = FAST (Shows only time averaged forces on bead)

The screenshot shows a Java application window titled "Gas Properties (3.05)" with a menu bar (File, Help) and a title bar. The main window is titled "Physics of Tweezers" and displays a simulation of a yellow bead trapped in a red optical trap. The trap is represented by a red, hourglass-shaped region. A yellow bead is positioned in the center of the trap. A "Return Bead" button is located on the left side of the trap. The right side of the window contains a control panel with various settings. At the bottom, there is a status bar with a clock, a "Play" button, a "Pause" button, a "Step" button, and a "Help!" button. The status bar also displays "3.66 fs".

Return Bead

Pops up when bead goes off screen.

Simulation speed

Slow Fast

Fields and Charges

☐ Show Laser's Electric field

Simulation Speed too fast to show

Forces on Bead

☐ Show Optical Trap Force

Horizontal trap force:

☐ On whole bead

☐ On each half

☐ Show Fluid drag force

☐ Show Brownian force

☐ Show Ruler

☐ Show Position Histogram

Advanced Features >

CAUTION

Laser ☐ on ☐ off ☐ freeze

Laser Power ## mW

3.66 fs

Play Pause Step Help!

Java Application Window

Given range ... slider likely should be logarithmic

Allow user to grab bead and move it around and release it from any point (confined to liquid).

Bead should have 3D shading.

This clock changes as sim speed changes ...
on "slowest Sim speed" 10 sec real time = 2×10^{-15} secs in sim time.
on "fastest Sim speed" 1 sec real time = 0.1 secs in sim time. (??)

Allow user to grab base of laser and move it left-right. Speed of movement should depend on "Sim speed" ... if on slow then restrict rate of movement so as not to exceed some reasonable rate (xx nm/sec).

Physics of Tweezers

Sim speed = FAST (Shows only time averaged forces on bead)

Question: Will this be interpreted correctly without x-y graph coordinates?

Background semi-transparent so can see bead if it goes behind.

Start and Stop button for position measurements. Clear button for histogram.

Simulation speed

Histogram of bead positions ... builds up over time (auto-scale this). (1 measurement every xx seconds).
Design issue: histogram really only makes sense at fast sim speeds.

Position Measurements

of measurements=xx

Start Clear

Fields and Charges

☐ Show Laser's Electric field

Simulation Speed too fast to display charges and fields

Forces on Bead

☐ Show Optical Trap Force

Horizontal trap force:

☐ On whole bead

☐ On each half

☐ Show Fluid drag force

☐ Show Brownian force

☐ Show Ruler

☐ Show Position Histogram

Advanced Features >

Return Bead

Pops up when bead goes off screen.

CAUTION

Laser ☐ on ☐ off ☐ freeze

Laser Power ## mW

3.66 fs

Play Pause Step

Help!

Show ruler brings up a ruler that tracks the beads x-position and shows the scale (bead ~200nm wide). Allow ruler to move vertically, but always keep it aligned with 0=center of laser.

Allow ruler to move up-down separate from histogram, which is not moveable, but have default as shown.

Physics of Tweezers

Sim speed = SLOW (show E-field and charges.)

The screenshot shows the 'Physics of Tweezers' simulation window. The main area displays a red laser trap with a yellow bead in the center. The simulation speed is set to 'Slow'. The 'Fields and Charges' panel is active, showing options for 'Show Laser's Electric field', 'Show Charges in Bead', 'All charges', and 'Excess charges'. The 'Forces on Bead' panel shows options for 'Horizontal trap force', 'Show Fluid drag force', and 'Show Brownian force'. The 'Advanced Features' panel includes a 'Reset' button. The bottom status bar shows a time of 3.66 fs and buttons for 'Play', 'Pause', and 'Step'.

Return Bead
Pops up when bead goes off screen.

E-field displayed as vectors on even grid that maps laser area (as in radio wave sim). Fading and size changes with strength

If sim speed slow enough, then allow these options. Slow enough means: about 1 sec = 10-15 sec of sim time

Wavelength of laser shows up in e-field grid... what wavelength do folks trap at, or do we just use He-Ne wavelength since laser is shown as red here? He-Ne = 632 nm. Actually is IR: 1064 nm

Simulation speed
Slow Fast

Fields and Charges
☐ Show Laser's Electric field
☐ Show Charges in Bead
☐ All charges
☐ Excess charges

Forces on Bead
☐ Horizontal trap force:
☐ On whole bead
☐ On each half
☐ Show Fluid drag force
☐ Show Brownian force

Advanced Features >

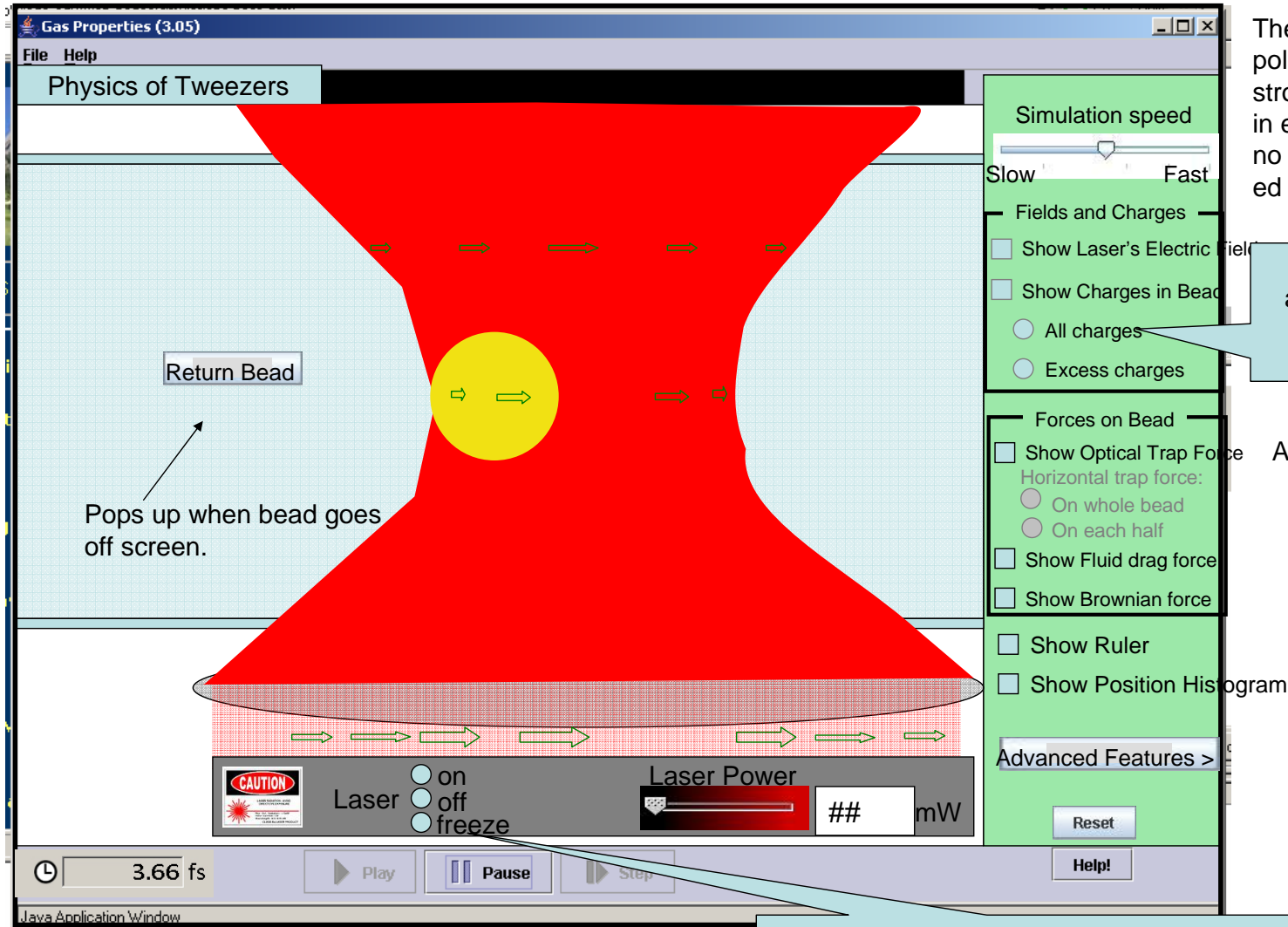
CAUTION
Laser ☐ on ☐ off ☐ freeze
Laser Power mW

3.66 fs

Java Application Window

Physics of Tweezers: Page 1

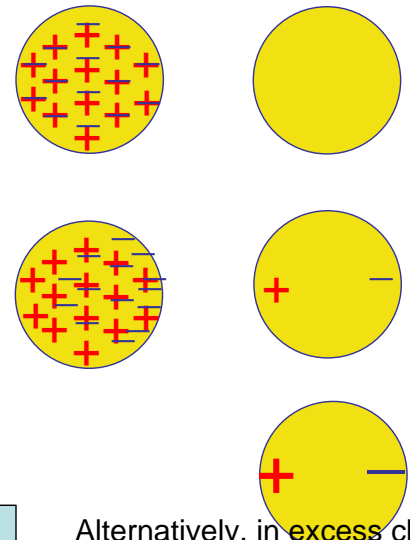
Sim speed = SLOW (show E-field and charges.)



The extent to which the bead is polarized will depend on electric field, stronger = more polarized. So as “zero” in e-field passes through, you will see no polarization. This will be Hollywooded since we only want qualitative idea.

Show charges should put grid of + and - charges, with -'s that moves slightly with E-field (creating polarization):

All charge view: Excess charge view:

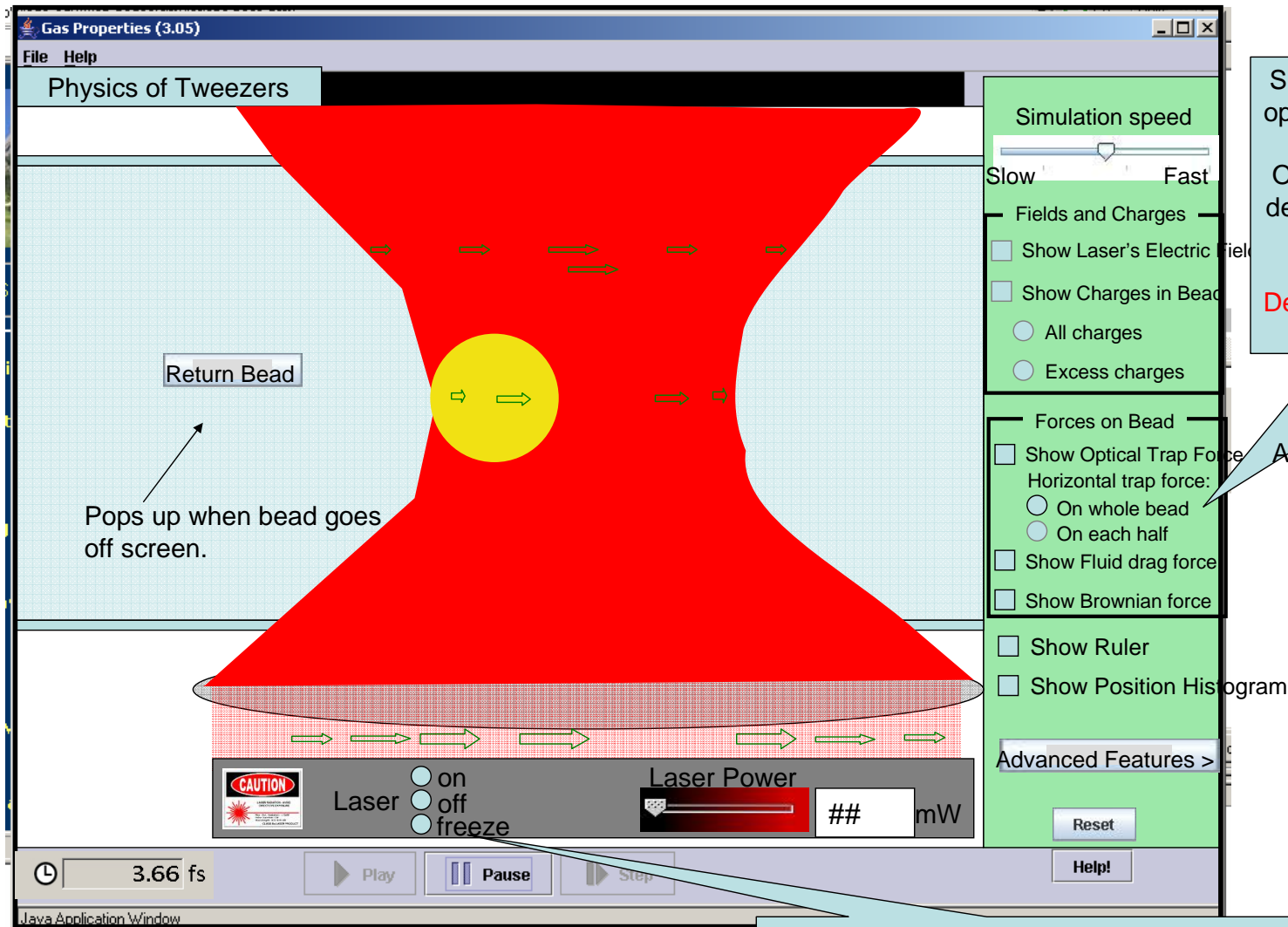


Should be able to pause or freeze laser and move bead about to see how charges and forces are different depending where you are in the beam.

Alternatively, in excess charge view could show charges all same size but more on each side as excess charge increases.

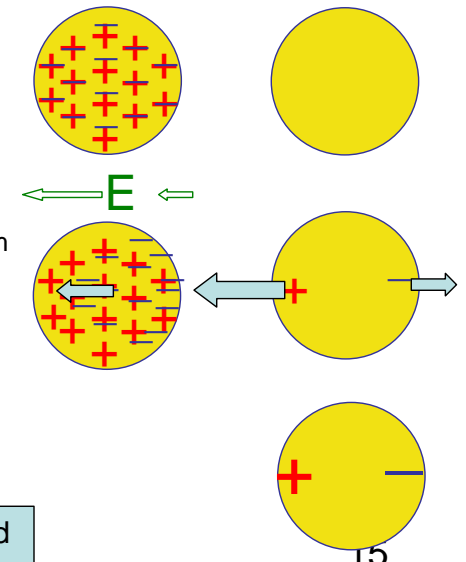
Physics of Tweezers

Sim speed = SLOW (show E-field and charges.)



Showing forces on bead... now these options are available (when sim speed is slow enough).
Optical trap force will grow and shrink depending on where you are in E-field wave cycle.
(Only show horizontal force ???
Detailed physics of vertical force is not apparent with this model)

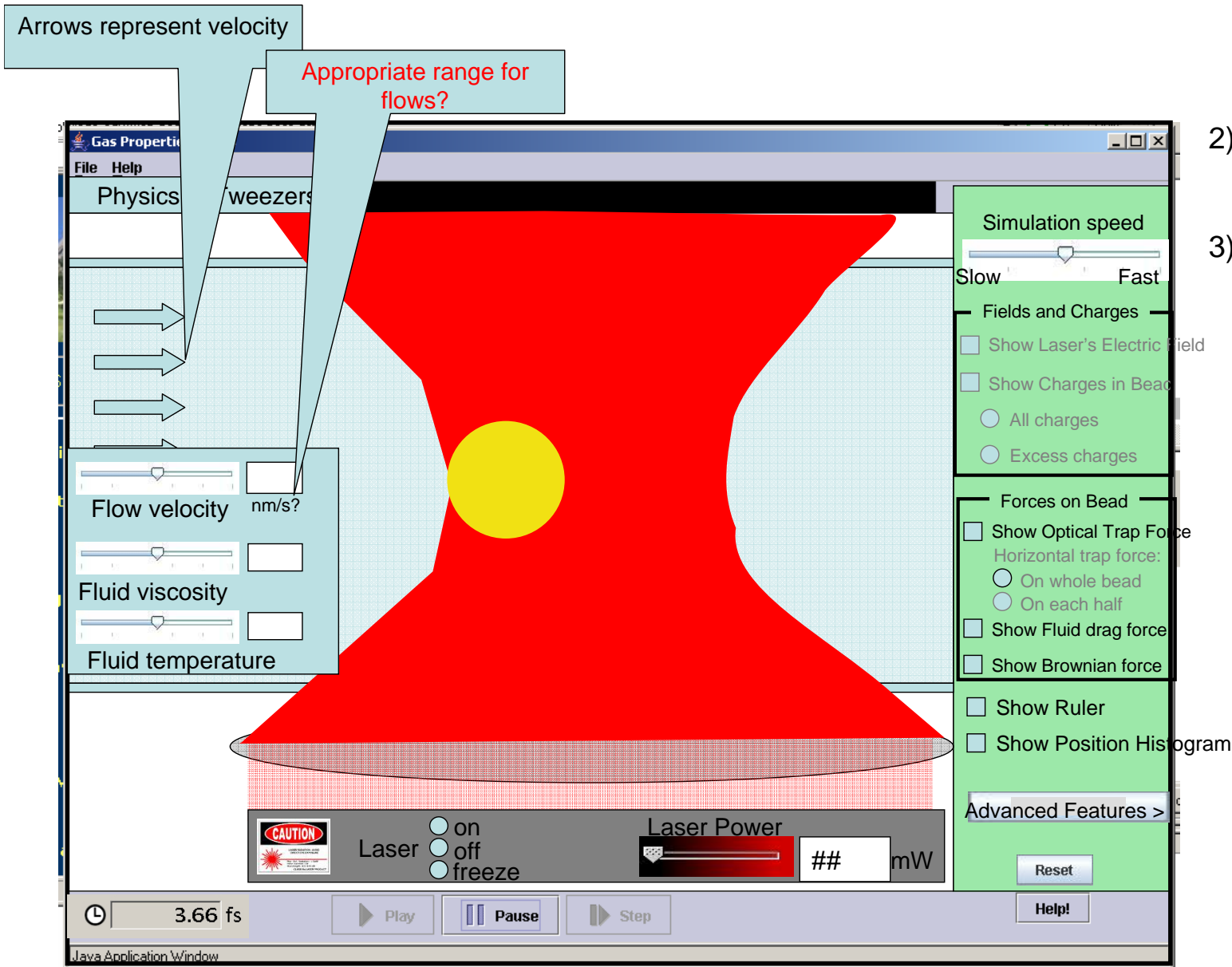
All charge view: Excess charge view:



Should be able to pause or freeze laser and move bead about to see how charges and forces are different depending where you are in the beam.

Physics of Tweezers

Sim speed = SLOW (show E-field and charges.)



- When any one of advanced options is selected then:
- 1) Sim speed skips to "fast" and if students try to readjust, does not allow student to go to slow speeds.
 - 2) Fields & charges grey out, Horizontal forces grey out.
 - 3) Bead and laser return to default location.

Advanced Features >

- ☐ Control Fluid and Flow
- ☐ Show change in momentum model for trap force
- ☐ Show potential energy graph

If Control Fluid and Flow selected, options at left appear:

$$F_{\text{drag}} = \gamma \cdot \text{velocity}$$

$$\gamma = 6 \pi \eta r$$

(η = viscosity ... will be adjustable).

r = radius of bead (not adjustable)

v = velocity of fluid relative to bead.

Temperature, will adjust F_{brownian} .

Physics of Tweezers: Page 1

Need good model of F_{trap} in this region

Physics of Tweezers

Potential energy of Trap

position

Return Bead

Pops up when bead goes off screen.

CAUTION

Laser ☐ on ☐ off ☐ freeze

Laser Power ## mW

Simulation speed

Slow Fast

Fields and Charges

☐ Show Laser's Electric field

Simulation Speed too fast to display charges and fields

Forces on Bead

☐ Show Optical Trap Force

Horizontal trap force:

☐ On whole bead ☐ On each half

☐ Show Fluid drag force

☐ Show Brownian force

☐ Show Ruler

☐ Show Position Histogram

Advanced Features >

Control Fluid and Flow

Show Trap potential energy graph

Show change in momentum model for trap force

If Show potential energy graph checked:

- 1) Graph appears at top
- 2) Curve shows $\frac{1}{2} k_{x_trap} x^2$
- 3) Little image of bead where bead is in x.
- 4) NO Units on PE curve

??? What to do with PE curve if person grabs bead and moves it up and down? Should whole curve shift up and down by appropriate amount? (That is k_{x_trap} is independent of x, but PE does go UP as bead moves vertically.).

Reset

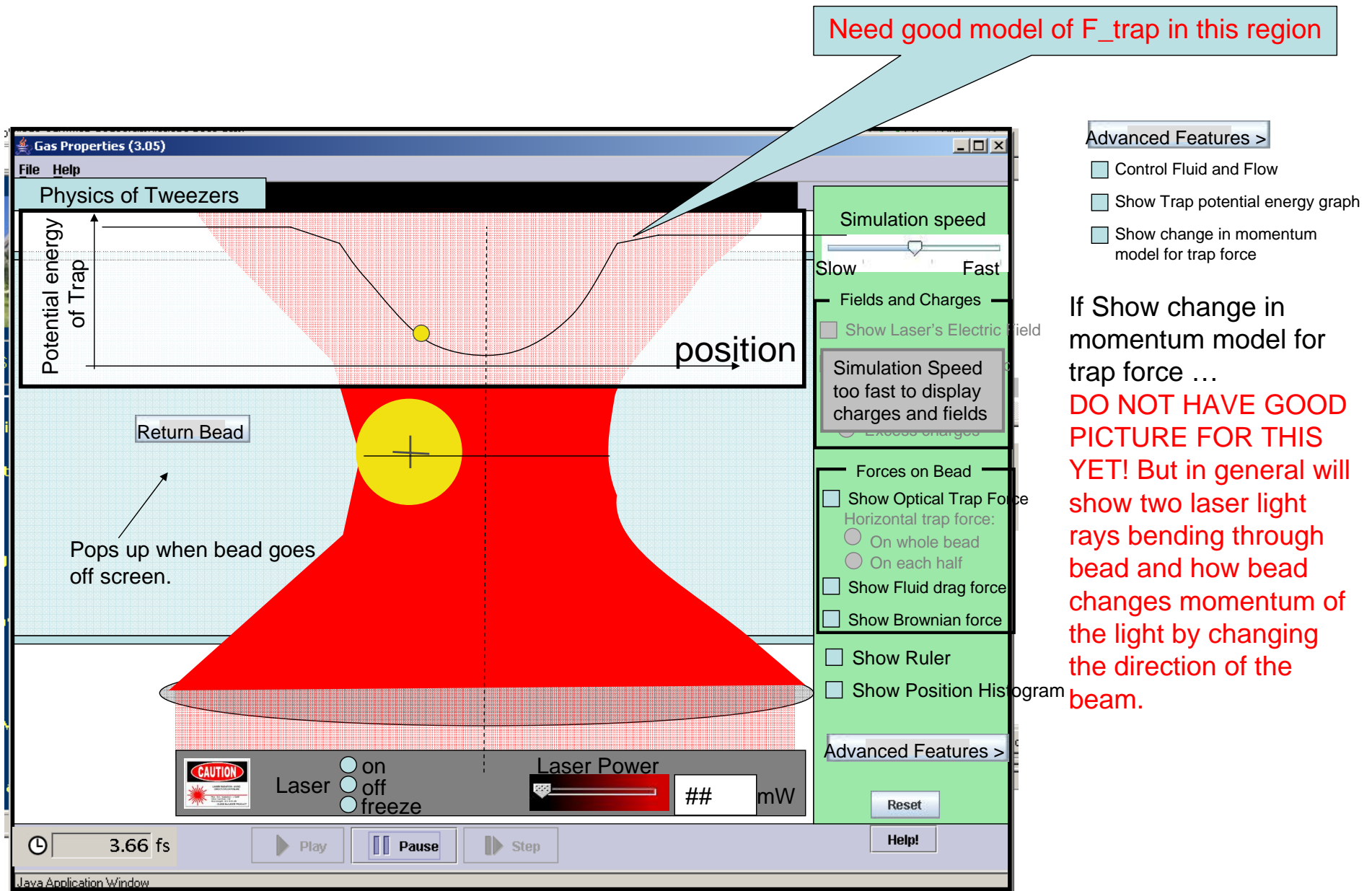
Help!

3.66 fs

Play Pause Step

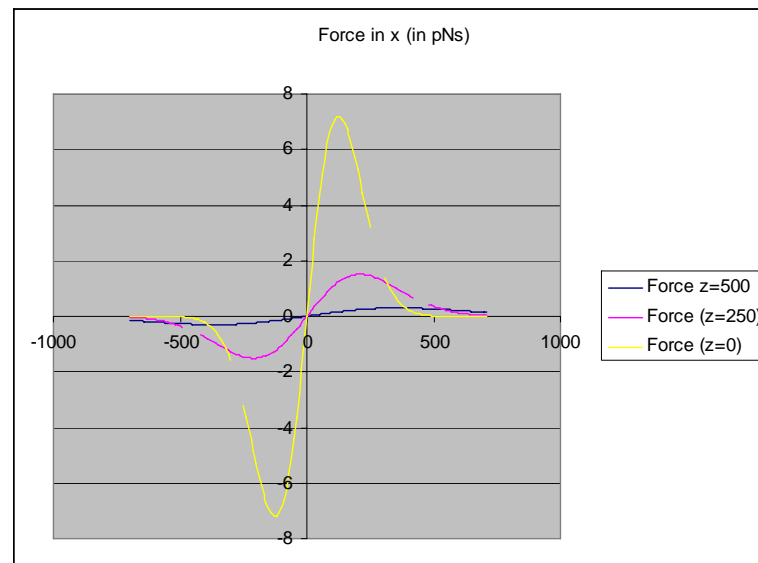
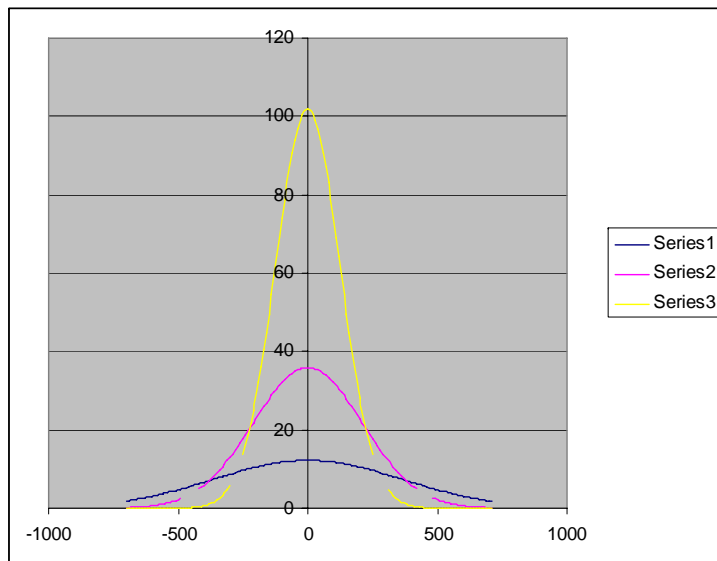
Java Application Window

Physics of Tweezers

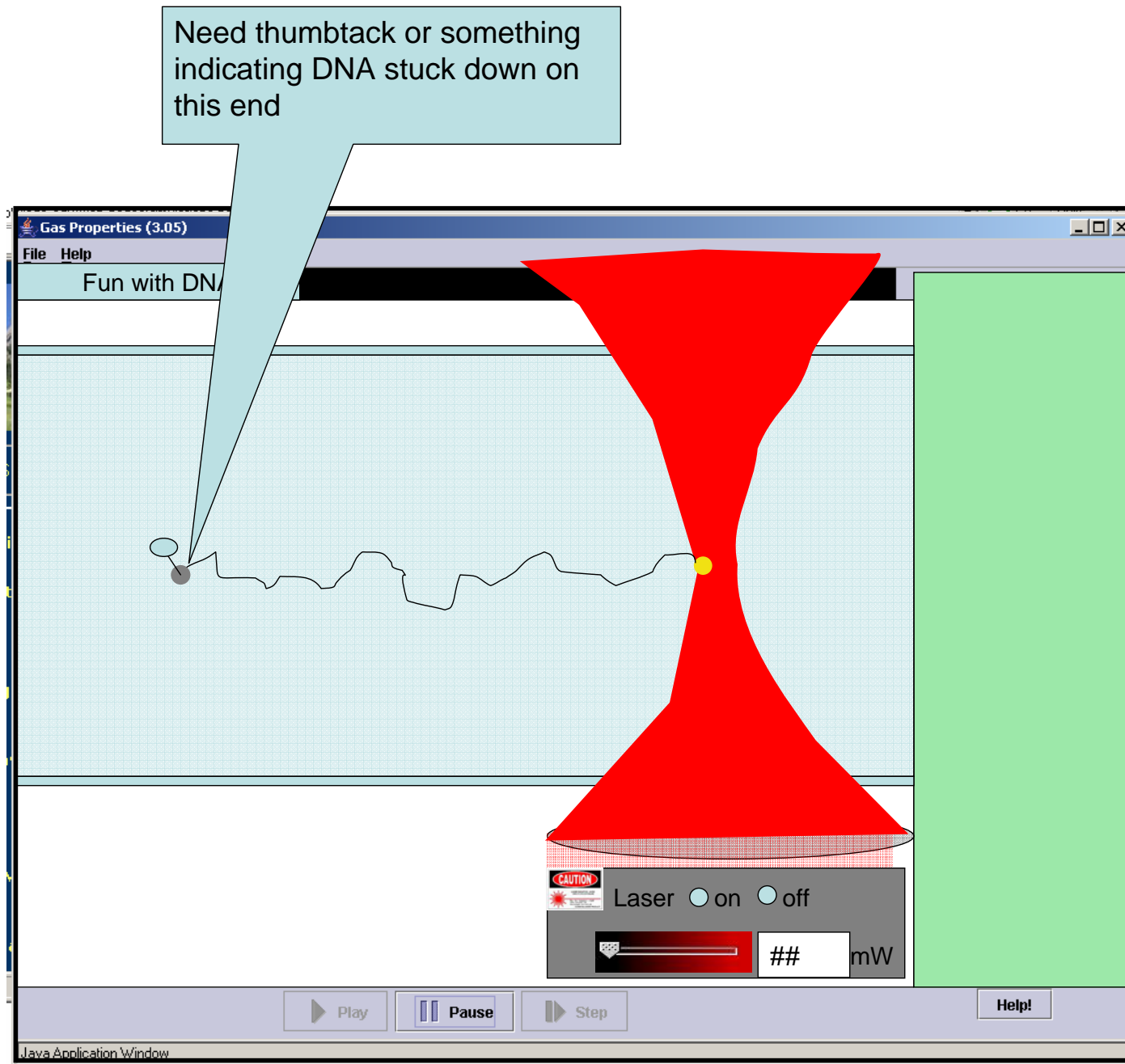


Models

- Laser beam profile ...
 - Model with hyperbola
 - Model shaded intensity with a gaussian
 - http://www.rp-photonics.com/gaussian_beams.html



Fun with DNA: Panel Two

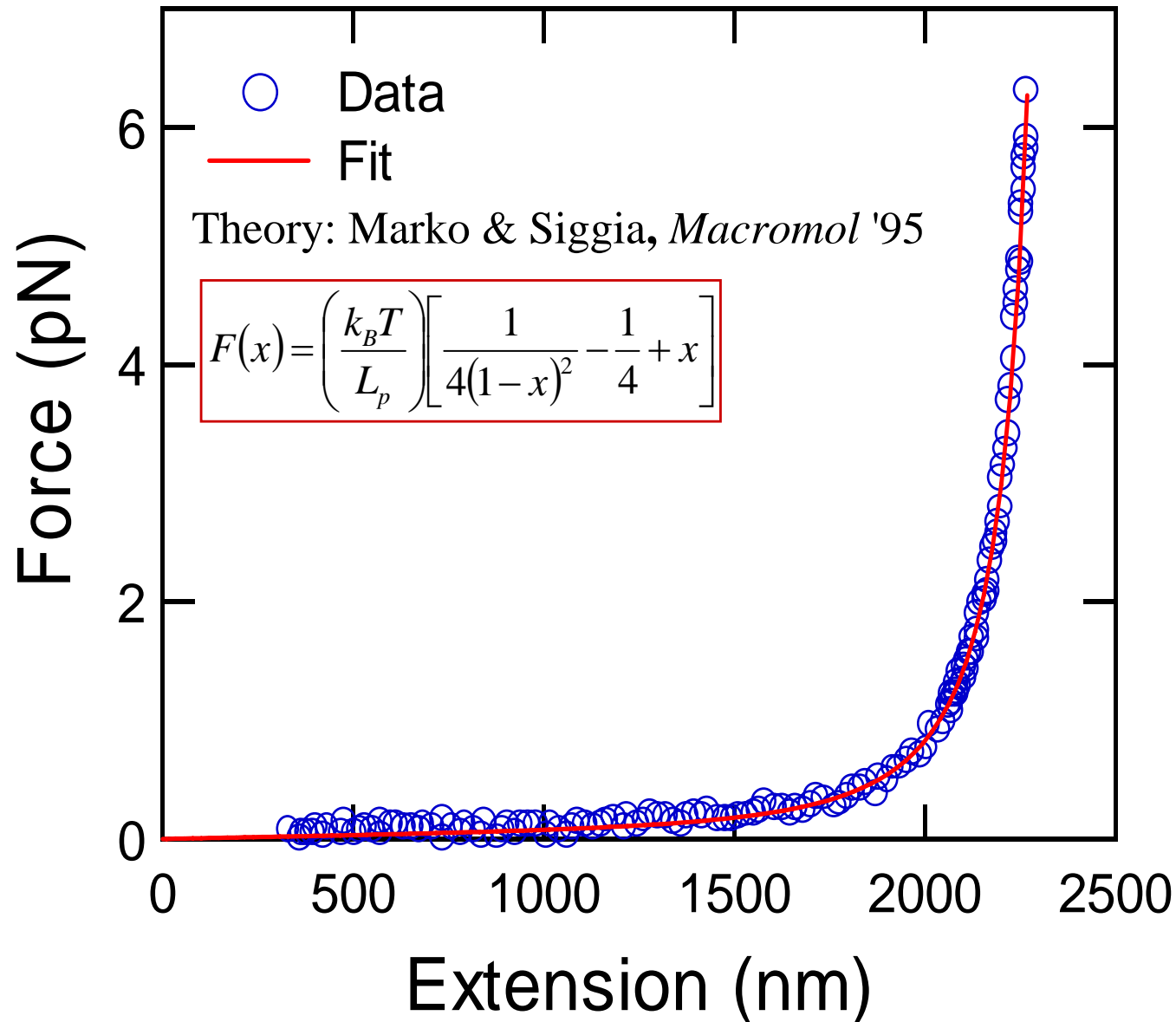


Basic idea:

- DNA with a bead on one end.
- Laser ON will trap bead.
- Can stretch DNA out ... it pulls back against F_{trap} on bead.
- If bead pops out of trap, see DNA recoil due to random walk.
- Same deal with viscous conditions, so $F_{\text{drag}} = \gamma \cdot v$
- Can manipulate bead directly with mouse, or by moving trap laser horizontally.

Single DNA molecules are well characterized

- Enables rate determination



Explanation of graph

k_B = boltzman constant

T = temperature in K

L_p = Persistence length (measure of bending stiffness)

... how long it looks straight for (50 nm for double stranded dna)

... single stranded dna ~1nm

$k_b T = 4.1$ pN-nm for 293K

$L_p = 50$ nm

So $k_b T = 4.1 * T/293K$ (gives pN-nm)

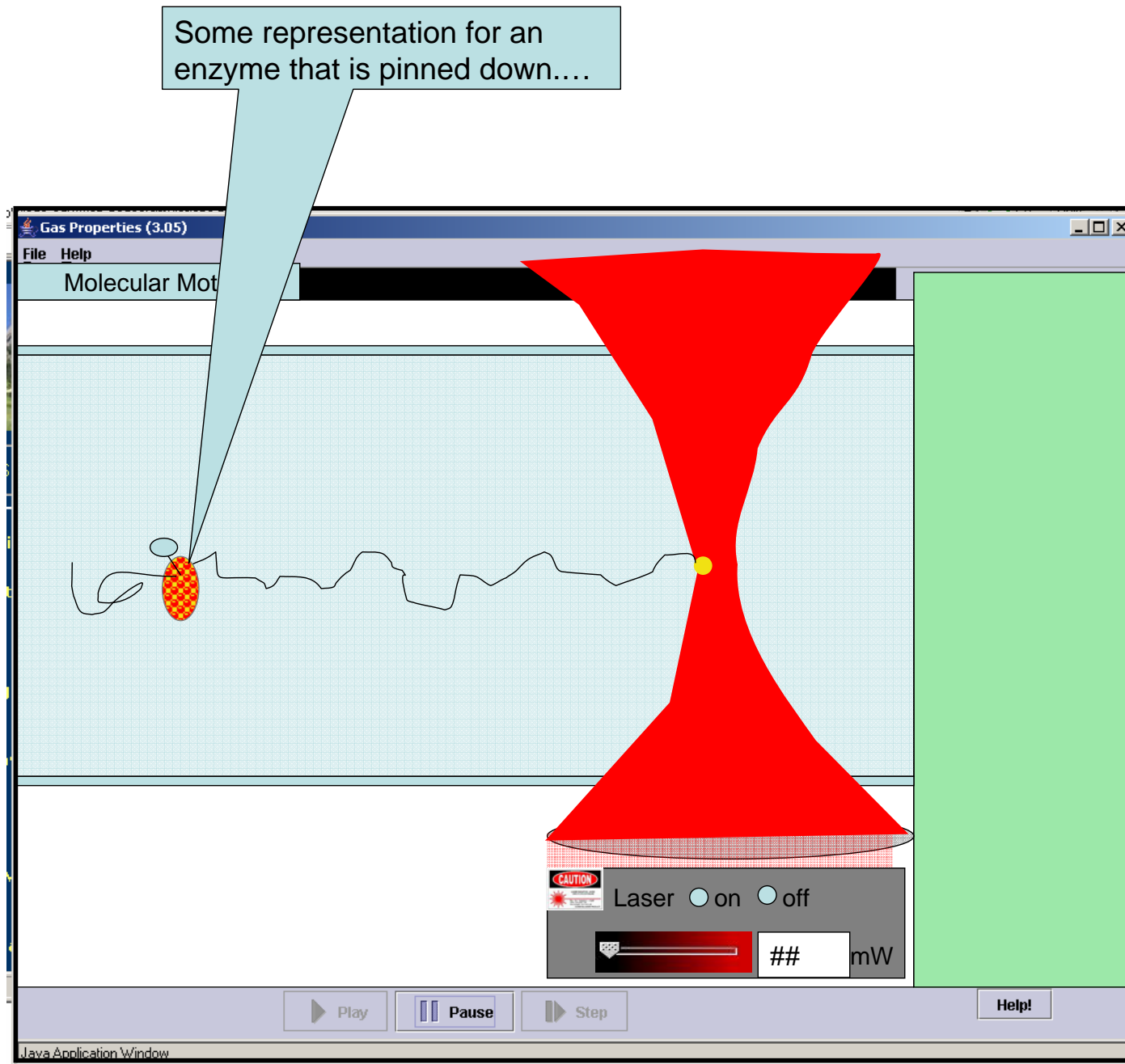
x = extension/total length of dna

= end-to-end between beads / contour length of dna

Picture shown for

2413 nm dna strand

Molecular Motors: Panel Three



Basic idea:

- Similar to DNA panel, accept now:

- Enzyme pulls on DNA (walks it to left) if ATP (food) is present.
- Force that enzyme pulls with can be measured using laser trap.

- Can now set trap to “maintain constant force” so that it tracks RATE at which enzyme moves DNA along.

Molecular Motors: Panel Three

Basic idea:

- Similar to DNA panel, accept now:
- Enzyme pulls on DNA (walks it to left) if ATP (food) is present.
- Force that enzyme pulls with can be measured using laser trap.

Remove controls:

- 1) Fluid flow

New controls:

- 1) ATP level:

- Slider for ATP level;
- Start with trying arbitrary units between 0 and 10.
- Propose to have this in the fluid on the play area
- Tom: Is linear scale for this enough? Graphs show logarithmic scale, but I would prefer linear if the point is clear enough.

- 2) Button (of alternative) labeled “hold trap force constant” which if pressed changes to “stop holding trap force constant”

- Possible locations: in “Forces on bead” section OR on laser control panel (since this is what you would control to hold trap force constant)
- Requirements: if user changes something about the laser (grabs and moves it or changes laser power OR grabs and moves bead then button will toggle so no longer holding trap force constant ... this needs to be a big enough change that users notice! Button color changes or something.).

If this button is active AND enzyme is moving the DNA strand, then LASER itself would move appropriately in x to maintain the F_{dna} as being the same given change in contour length of the DNA molecule as the enzyme moves it. Knowing how far in x to move the laser is determined by keeping the following ratio constant:

ratio = extension/total length of dna

= end-to-end between beads / contour length of dna

So you'll have (end-to-end x distance)_new = (end-to-end x distance_old / contour length_old) * contour_length_new

And you'll want to move the laser over by:

end-to-end x distance _old – end-to-end x distance_new.

Forces from the enzyme's perspective:

-F_{dna} determines current “load” on enzyme.

-So, F_{dna} and ATP will determine velocity with which it moves DNA along

From bead's perspective:

-Bead model is the same as panel 2 (F_{dna} and F_{trap}) just that F_{dna} and F_{trap} will increase as the DNA moves through the enzyme.

Model:

Velocity of DNA moving through enzyme as function of [ATP] and F_{dna}

Also will need to go to 10x current max sim speed on this panel.

$$\text{Velocity} = V_{\text{Max}} * [\text{ATP}] / ([\text{ATP}] + K_M)$$

K_M is a function of the Force_{dna} (in pN)

V_{max} is a function of F_{dna} (in pN)

[ATP] goes from 0 to 10

$$V_{\text{max}} = d_2 * c_1 / (c_2 + c_3 * e^{(F * c_4)})$$

$$K_M = d_1 * (c_6 + c_7 * e^{(F * c_8)}) / (c_2 + c_3 * e^{(F * c_4)})$$

d₂ = 5000 nm/s (make this and others easily changeable)

d₁ 2.281

c₅ 2.1

c₆ 2

c₇ 0.1

c₈ 1.2

c₁ 4.79

c₂ 4.7

c₃ 0.09

c₄ 0.82

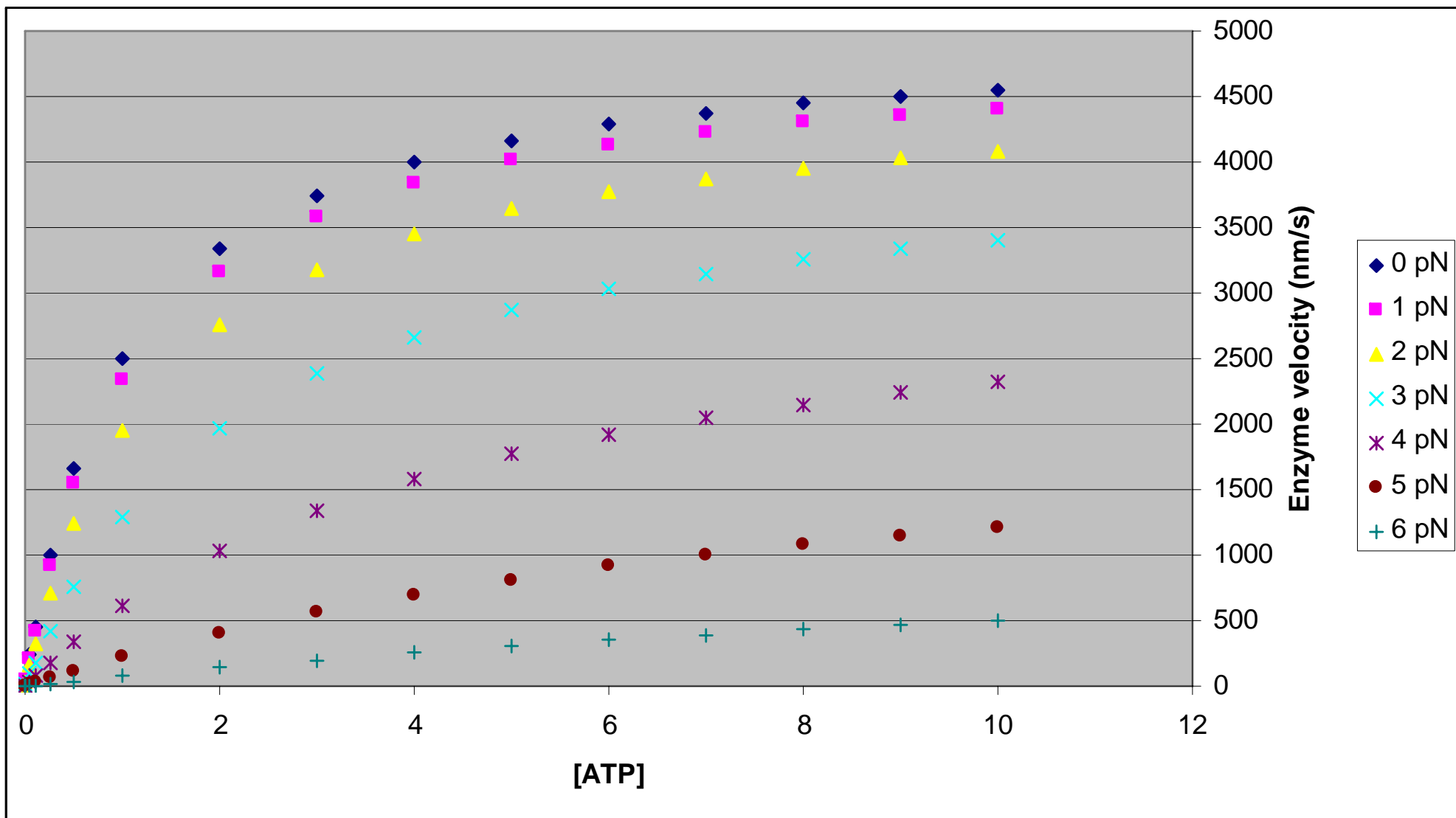
Where F is the dna force (either created using hand manipulation of bead or created using trap itself)

All of these parameters should be set up to make easy changes if needed ... we are not modeling an exact enzyme here, just trying to get the general dependencies correct.

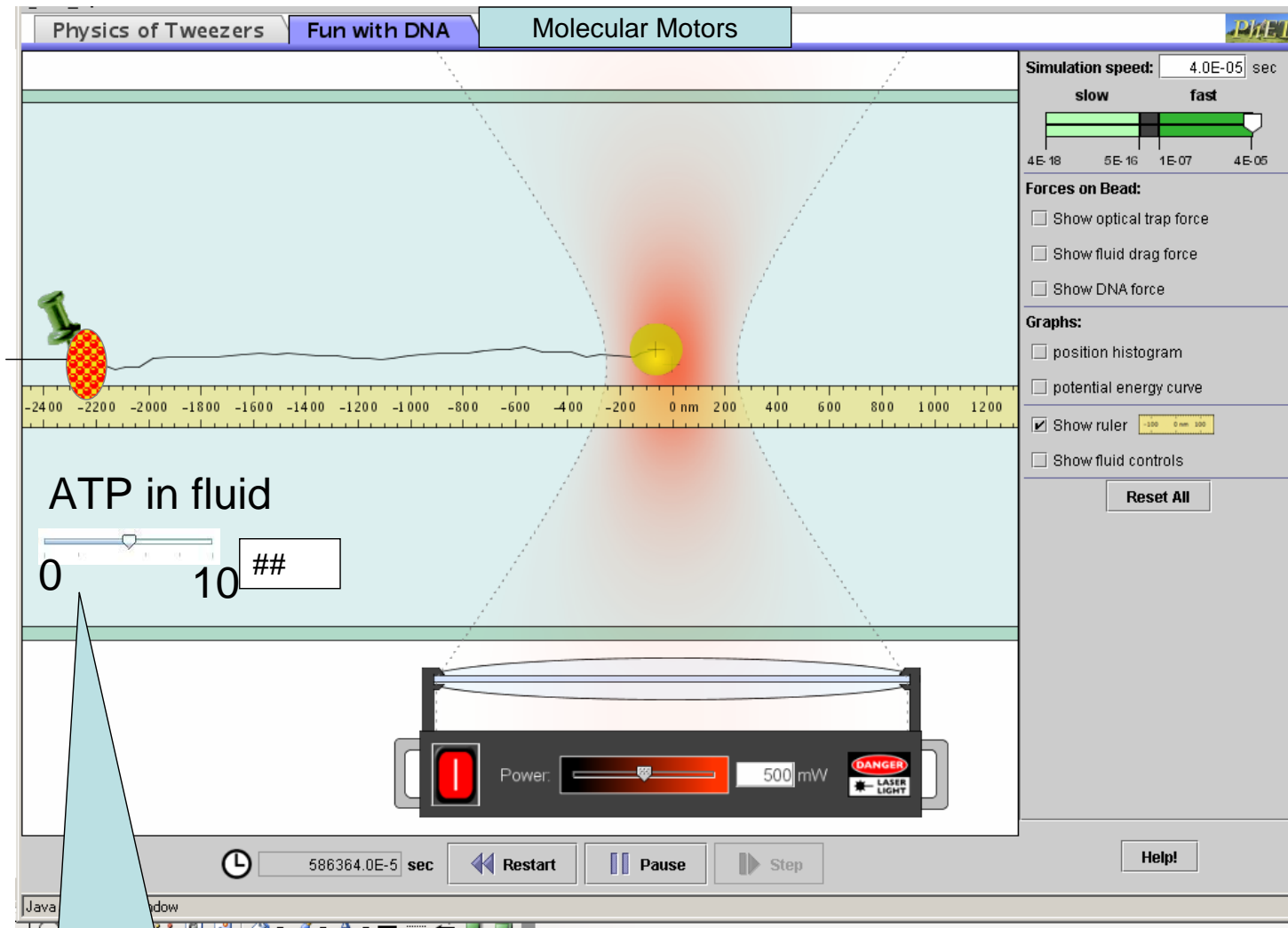
Velocity – decreases as load (trap force) increases

And velocity increases as ATP concentration increases.

ISSUE for TOM: we are not modeling the “stall” force (where the enzyme will just stop)
Stall force should depend on ATP concentration



Molecular Motors: Panel Three



Control ATP conc in fluid
... arbitrary units (may
possibly want real units in
end?)

Other issues Tom brought up:

Biochemical step vs mechanical step as rate limiting force

If biochemical is rate limiting, increase in force will not immediately change rate.