Title: Monte Carlo Simulations of the Interaction Between a Self-Avoiding Polymer and a Membrane

Date: Apr 23, 2009 04:00 PM

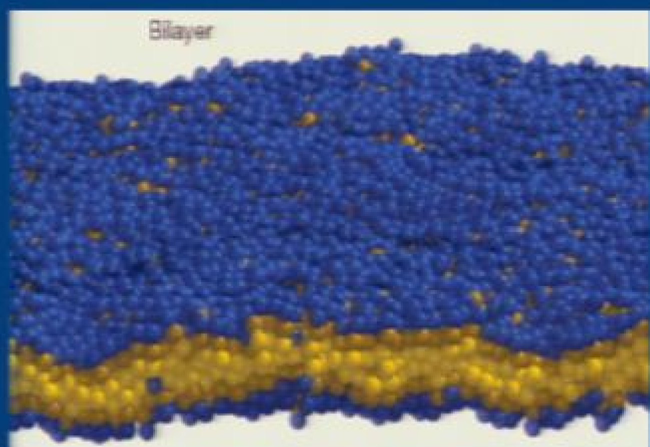
URL: http://pirsa.org/09040028

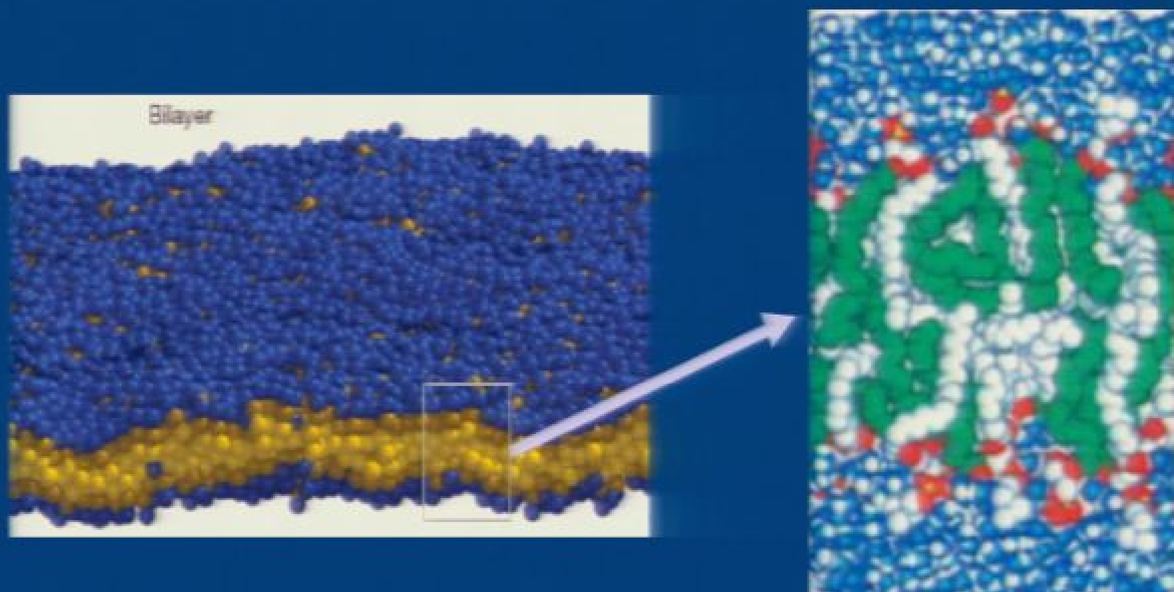
Abstract:

Structures of membranes interacting with macromolecules

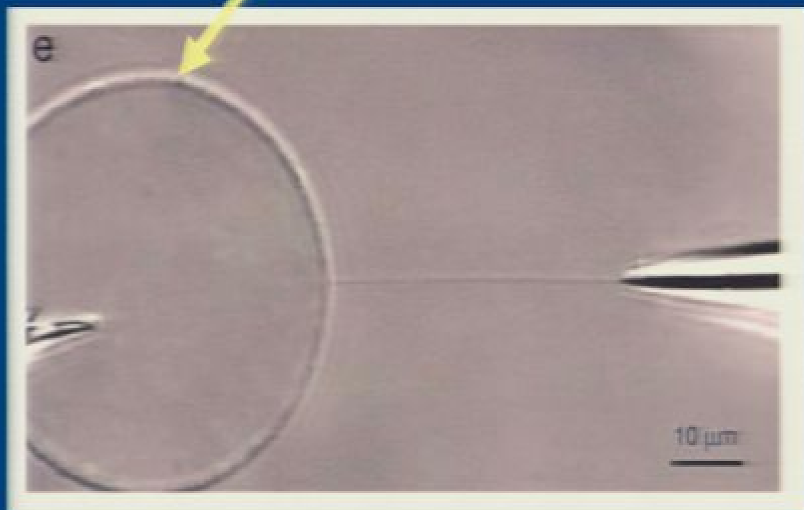
Jeff Z. Y. Chen
Department of Physics & Astronomy
University of Waterloo

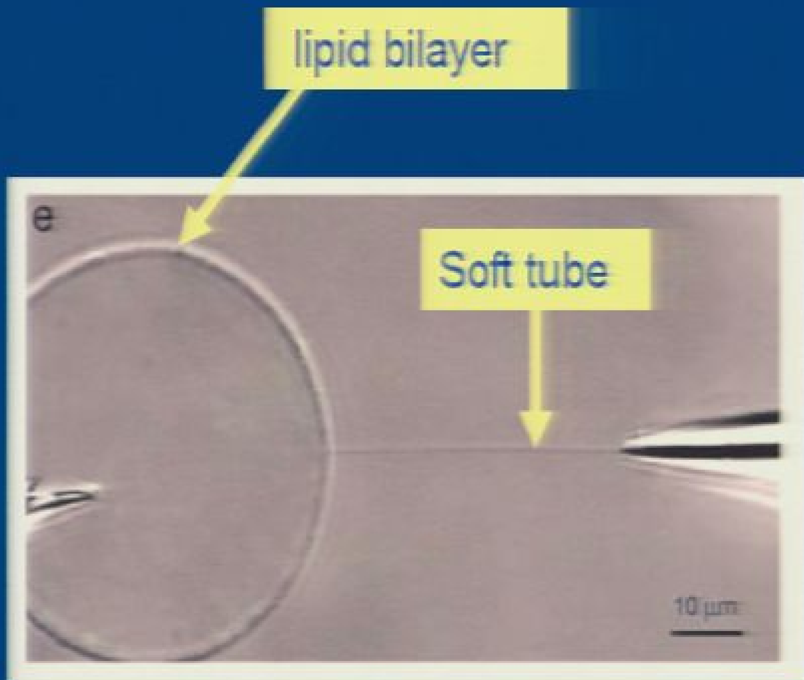
- Introduction to tubular membrane
- DNA confined in a soft tube
- Nanoparticles on a soft sheet


Bilayer


Bilayer

lipid bilayer





Experiments: membrane tubes

- Borghi, Rossier and Brochard-Wyart, Europhys Lett **64**, 837 (2003)
- Tokarz, etc, PNAS **102**, 9127 (2005)
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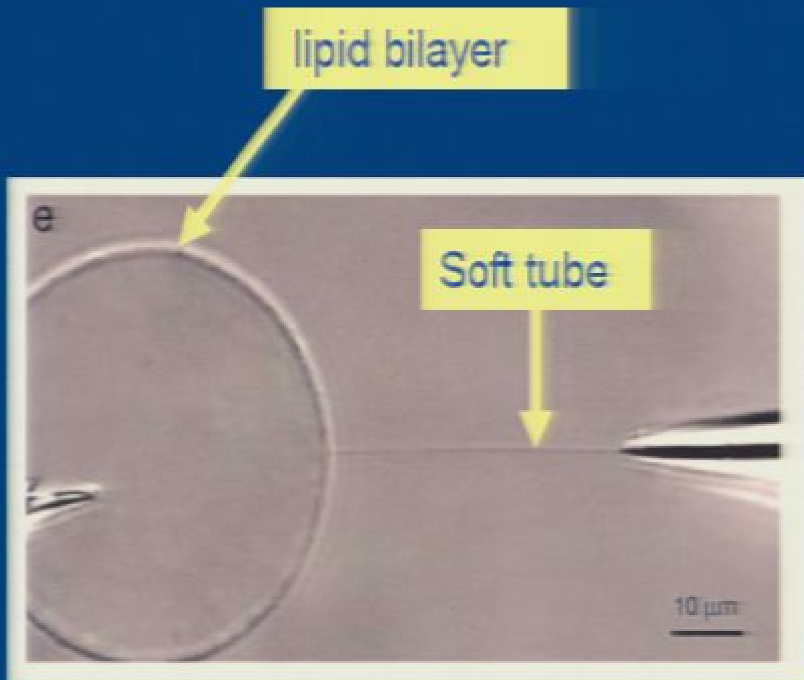

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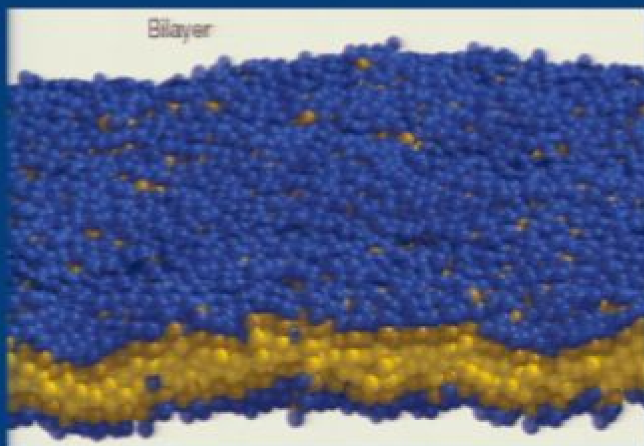
Energy model: **Helfrich model** for a fluid membrane



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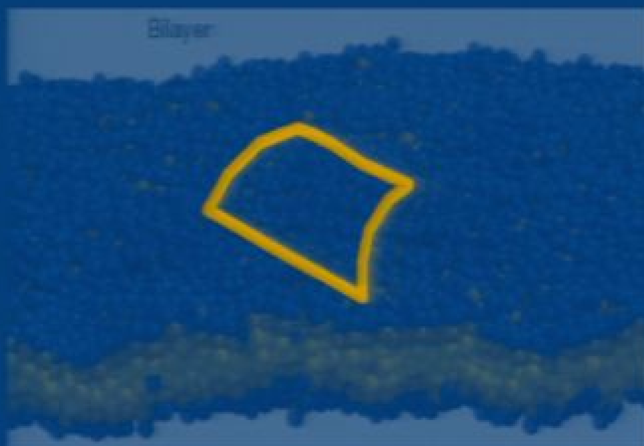

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- Physical parameters

  surface tension: σ

  bending energy: κ

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  - principal curvatures: $1/r_1$ and $1/r_2$
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Helfrich energy = $\Delta A \left[\sigma + (\kappa/2)\,(1/r_1 + 1/r_2)^2\right]$

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- $\beta\kappa = 20$
- $\sigma a^2/\kappa$: 10^{-3} to 10^{3}

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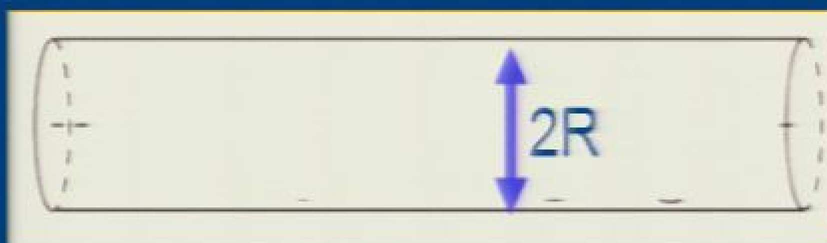

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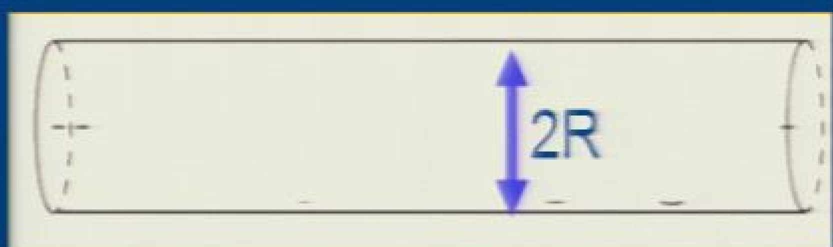

- $1/r_1 = 1/R$
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$$E = 2\pi L R\left[\sigma + \kappa/(2R^2)\right]$$

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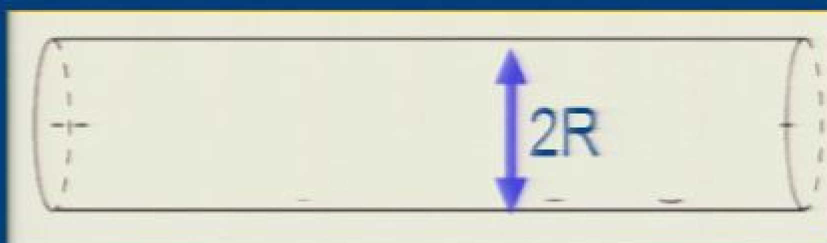

- $1/r_1 = 1/R$
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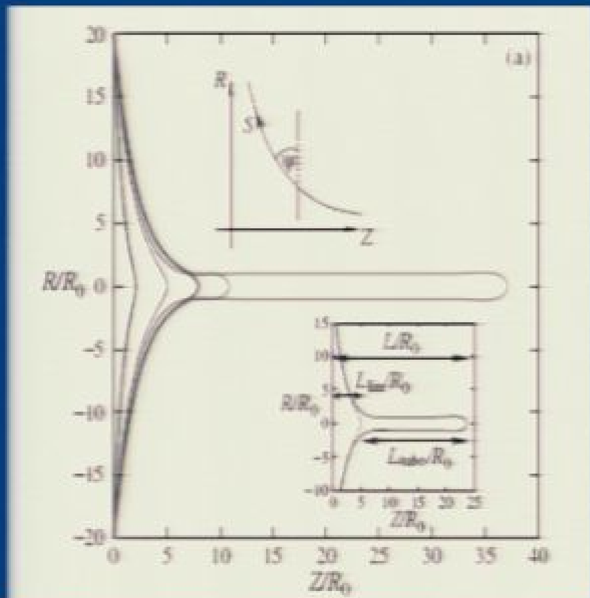
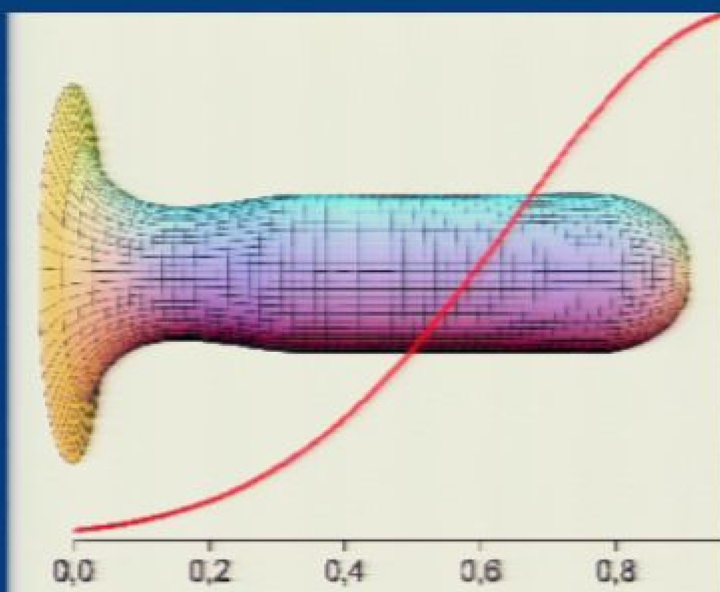
$E = 2\pi L R\,[\sigma + \kappa/(2R^2)]$

Minimization: $dE/dR = 0$

Equilibrium: $R_0^2 = \kappa/\mathbf{2}\sigma$



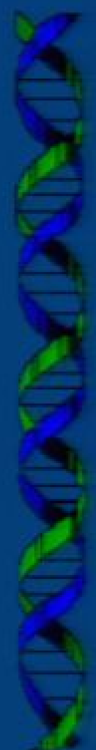
Derenyi, Julicher and Prost, PRL 88, 238101 (2002)

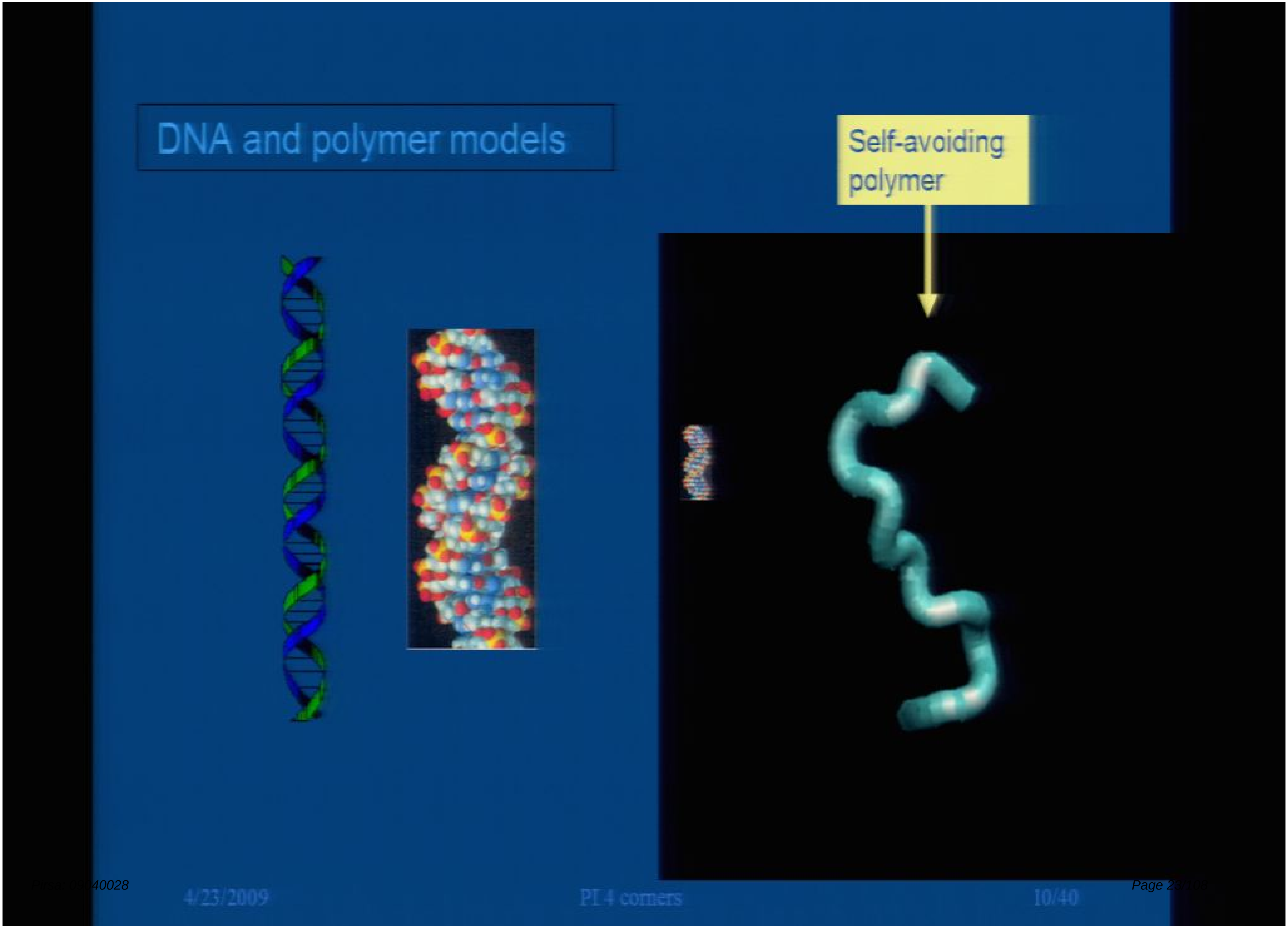


Campelo and Hernandez-Machado, PRL, 100, 158103(2008)

TOPIC 1: Swollen-to-globular transition of a self-avoiding polymer confined in a soft tube

DNA and polymer models




DNA and polymer models
Self-avoiding polymer
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PI 4 corners
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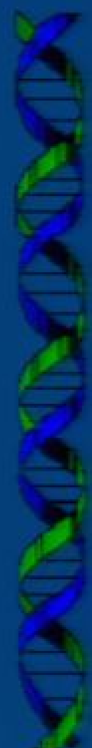
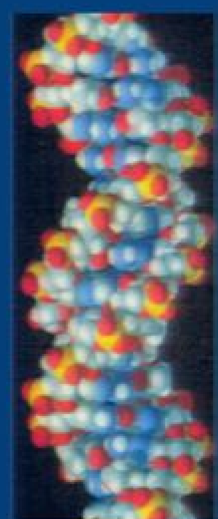
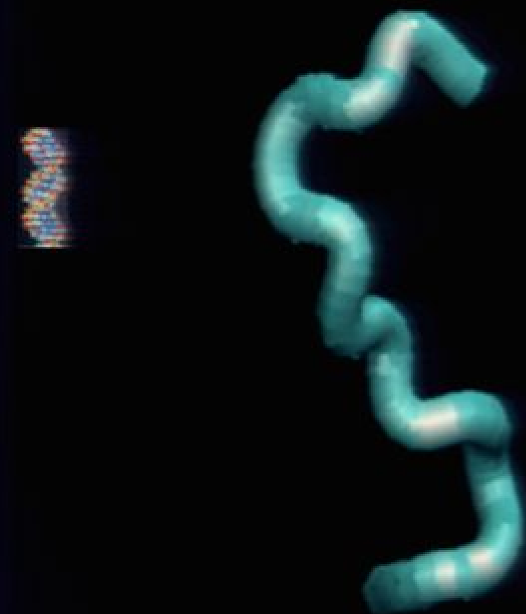
DNA and polymer models

Self-avoiding polymer

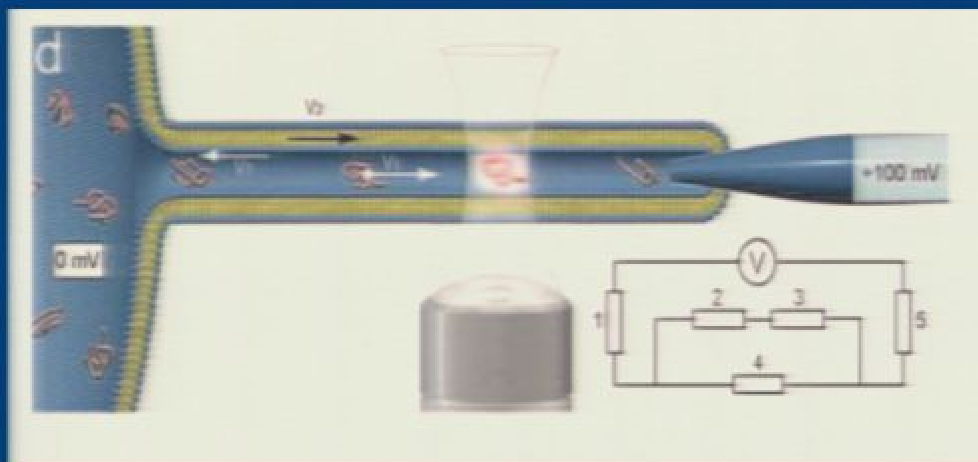






"DNA physics" ← Polymer physics

DNA in a soft tube



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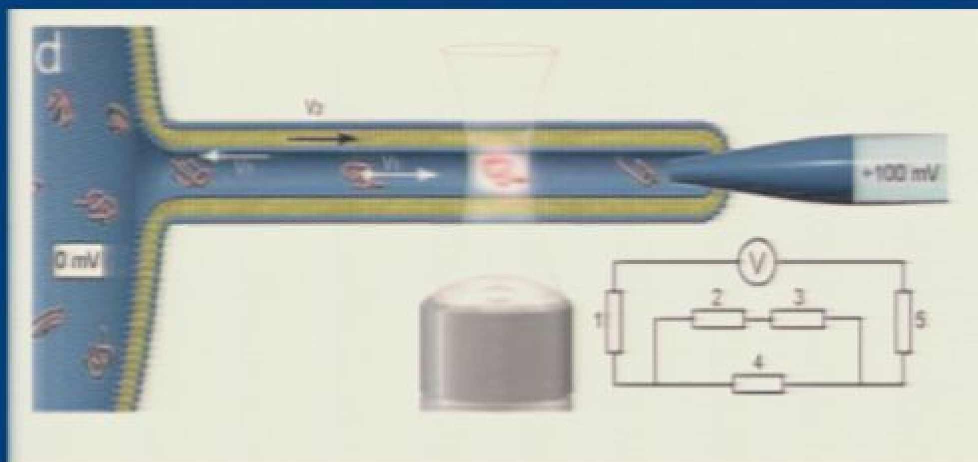

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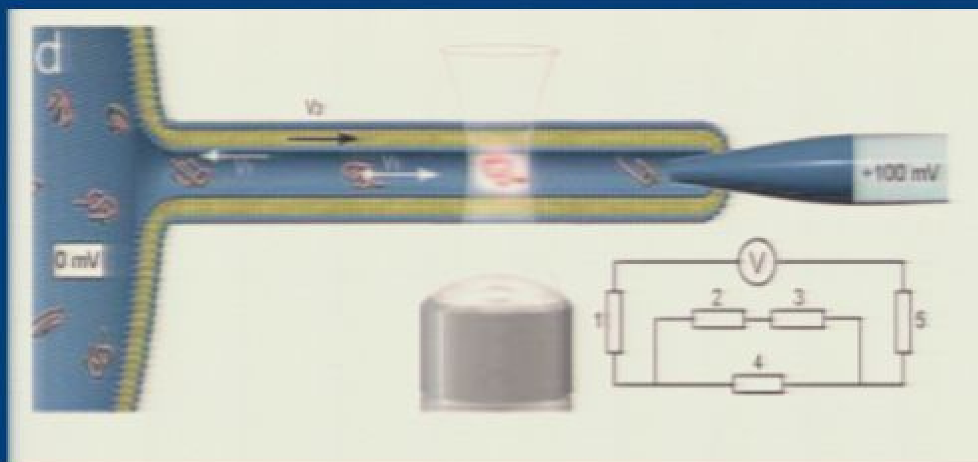

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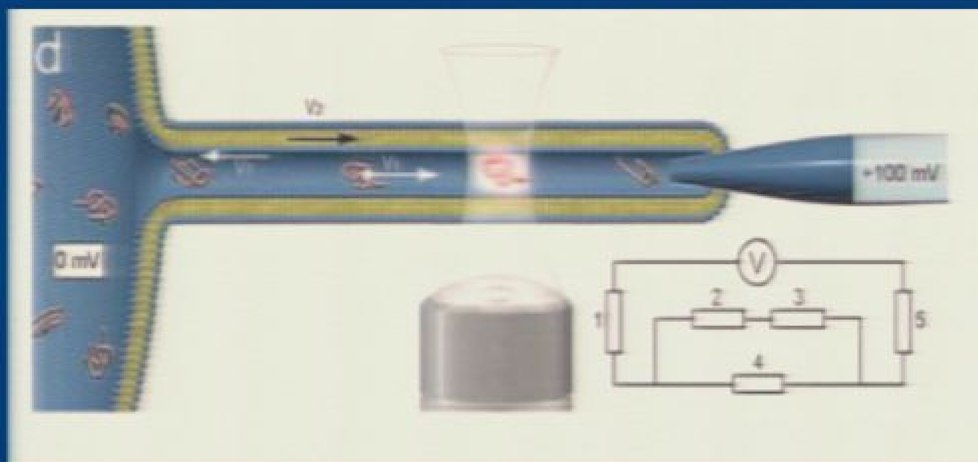

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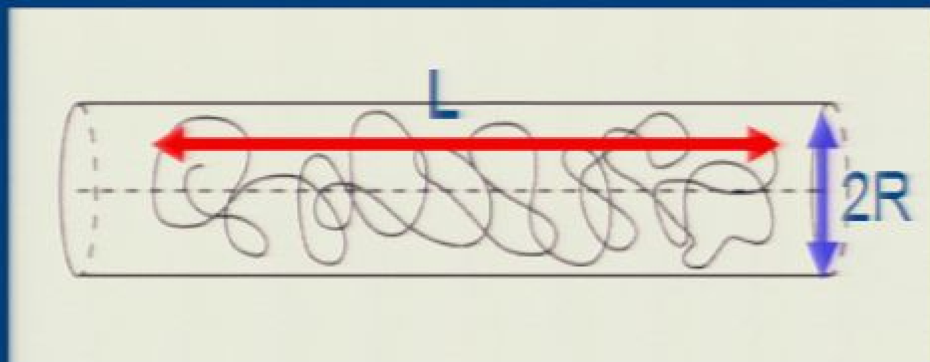
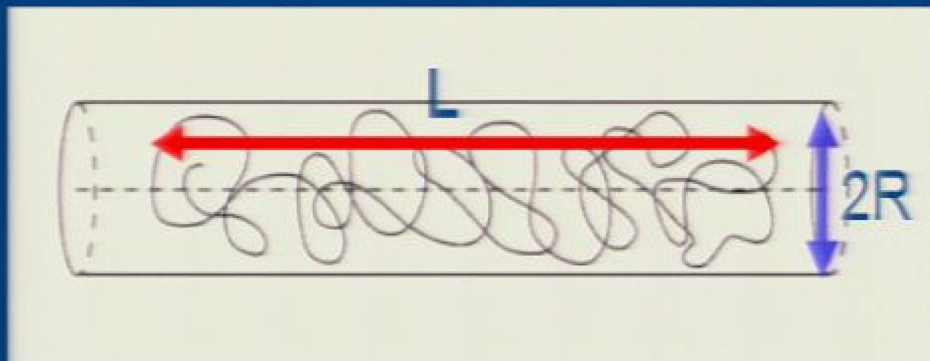
A self-avoiding polymer confined in a soft tube

Polymer confined in a hard tube



Polymer confined in a hard tube

Total polymer length N



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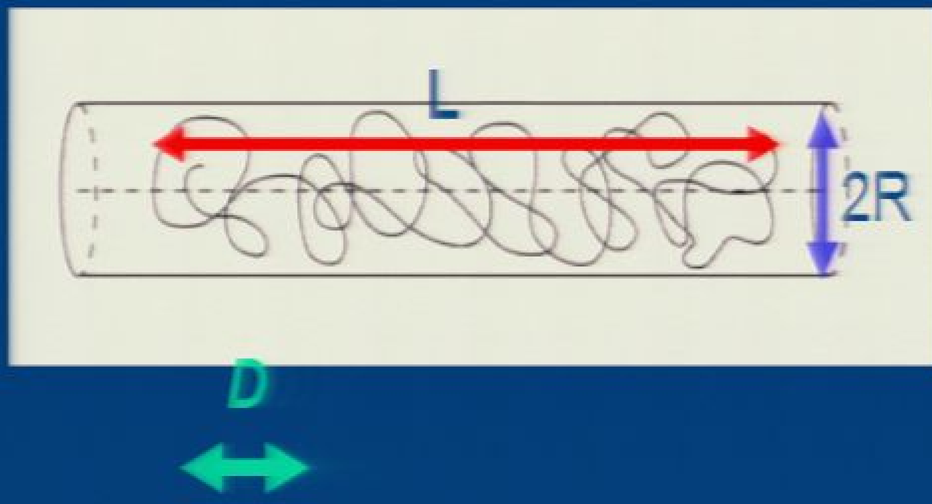
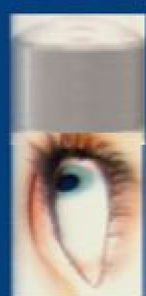


$$L = N\,R^{-2/3}$$



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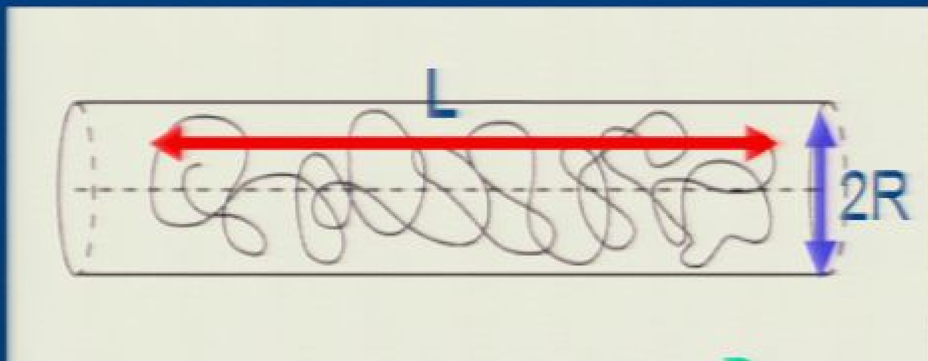

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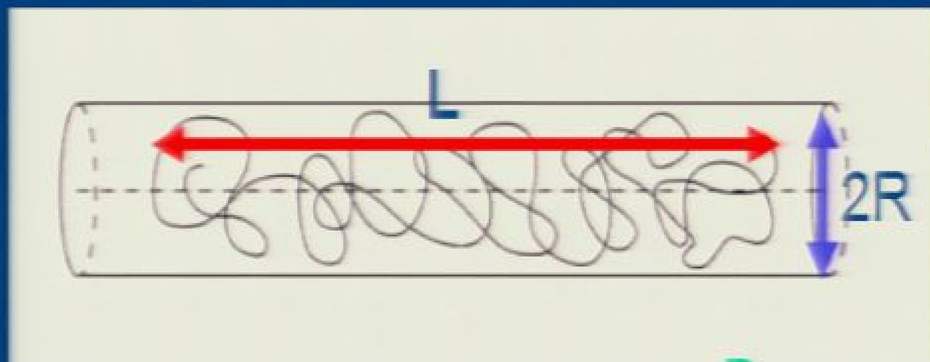

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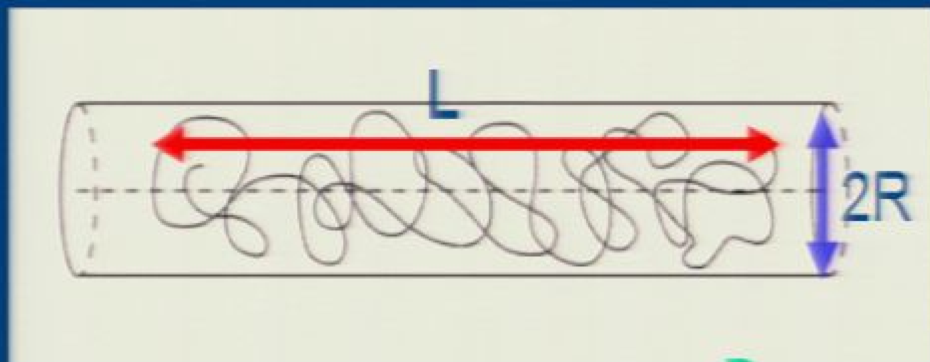

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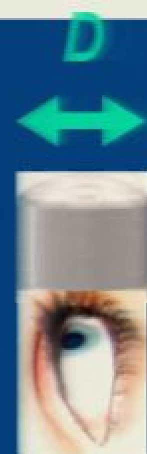
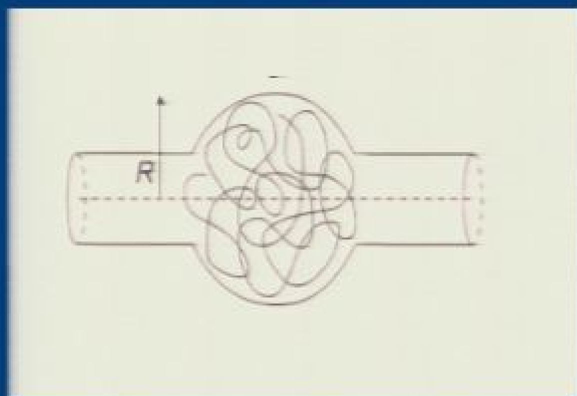


- Signal strength ~ D*R**2 * [N/(L*R**2)] = D*R**(2/3) = N-independent, weak
- However, signal strength ~ N experimentally in some cases.

Under what circumstance would signal strength ~ N ?



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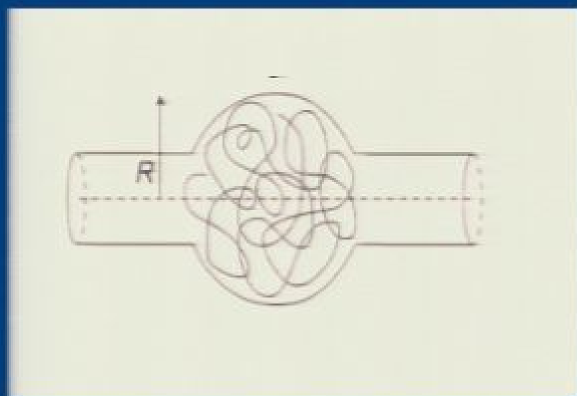

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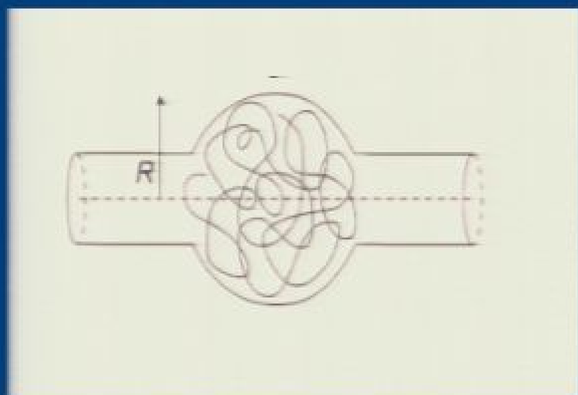

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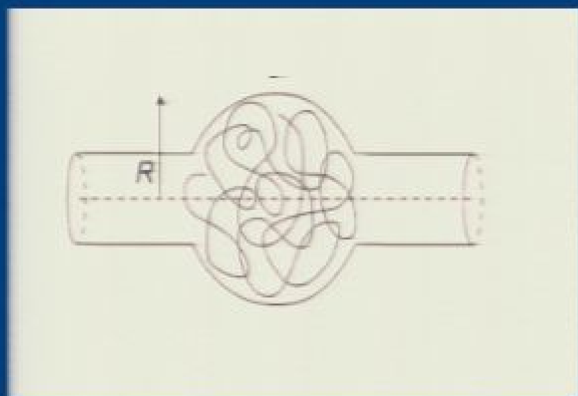

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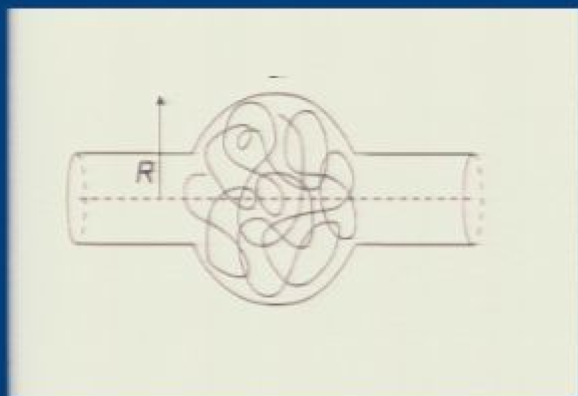

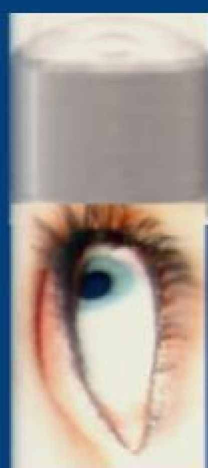

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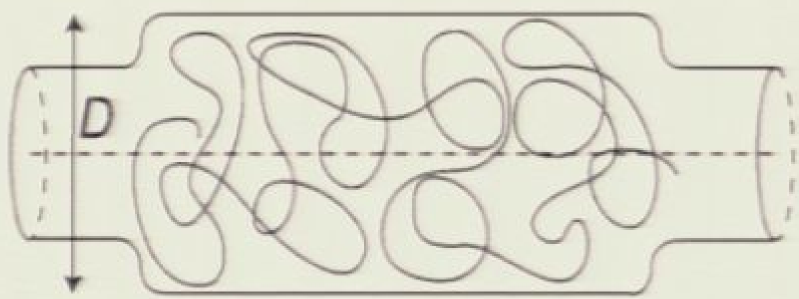
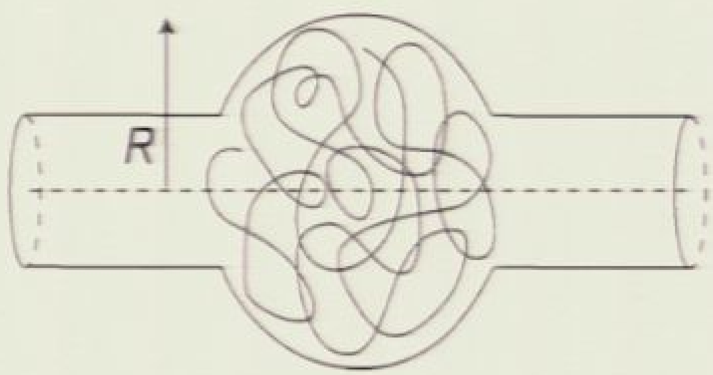
- Theory and simulation: simultaneous consideration of **polymer and soft tube.**

Swollen to globular transition



- Swollen (elongated)



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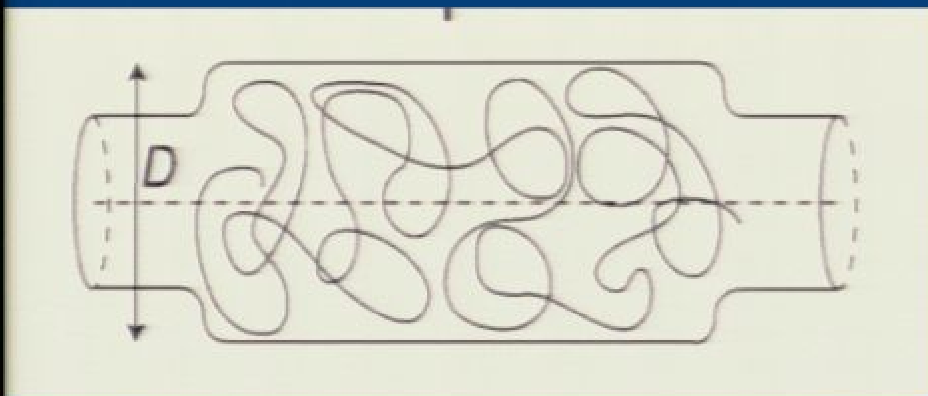
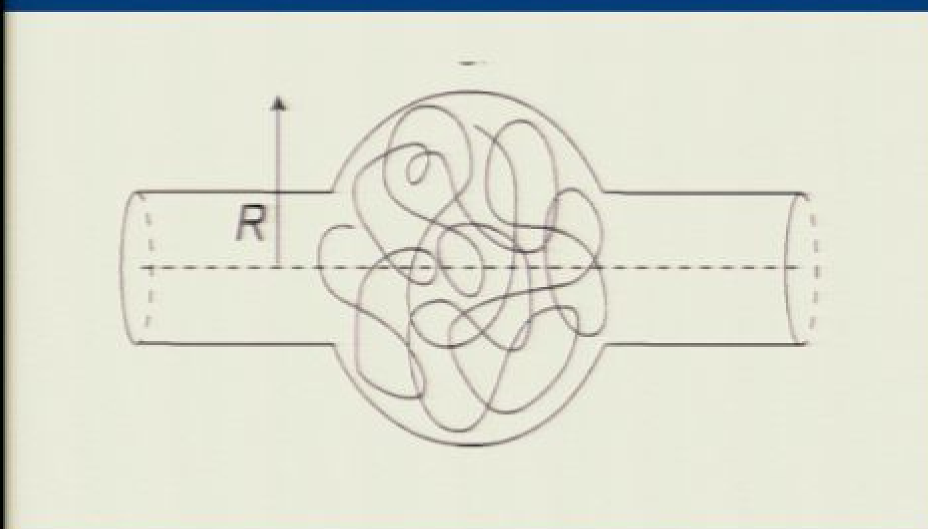
Swollen to globular transition



- Swollen (elongated) "Snake eating a swollen sausage (De Gennes)"



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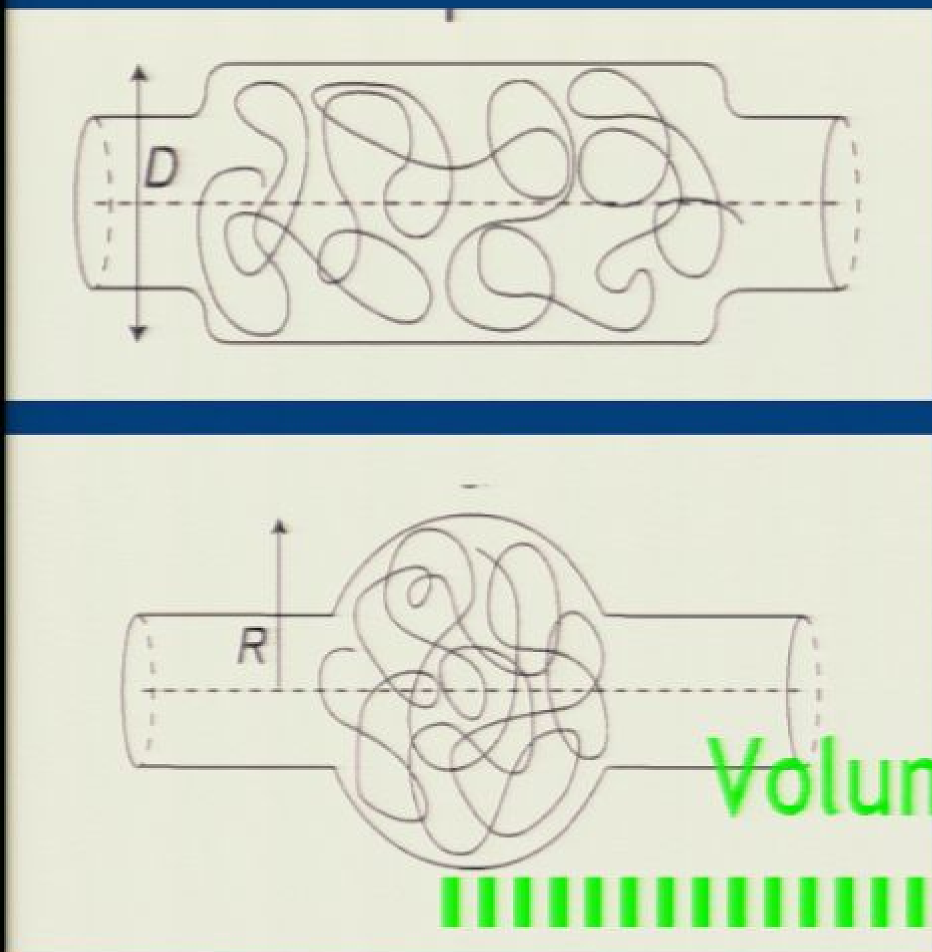

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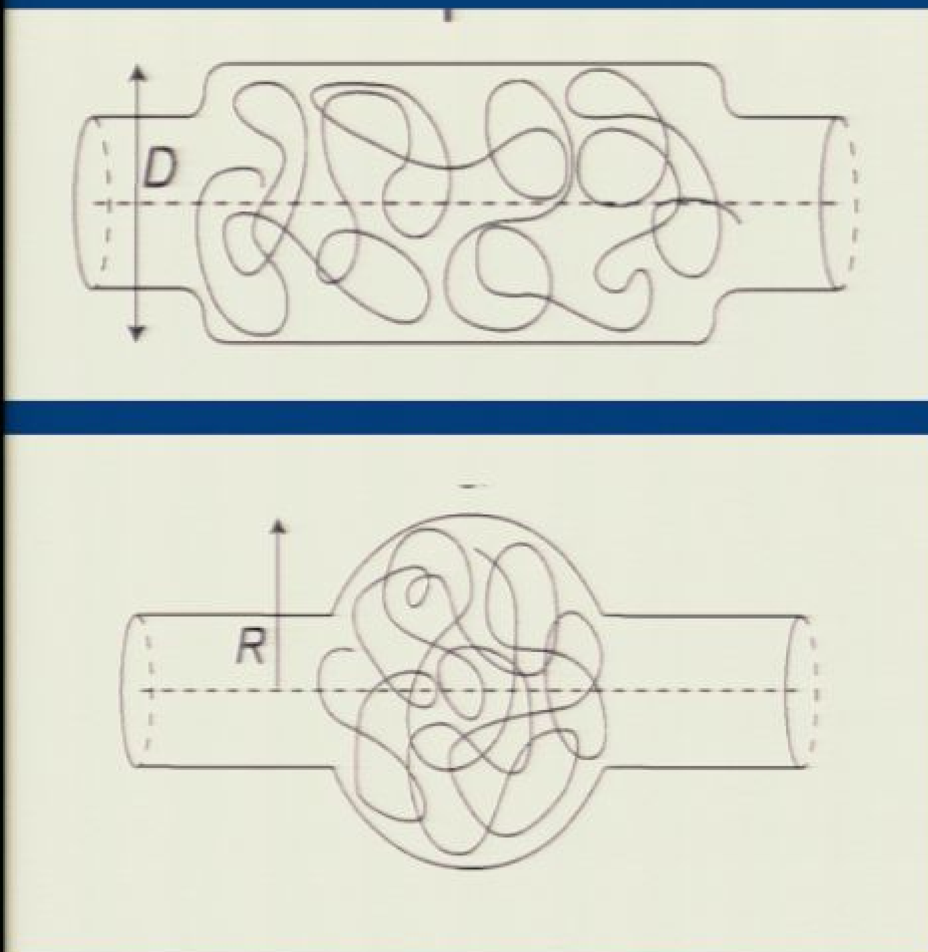

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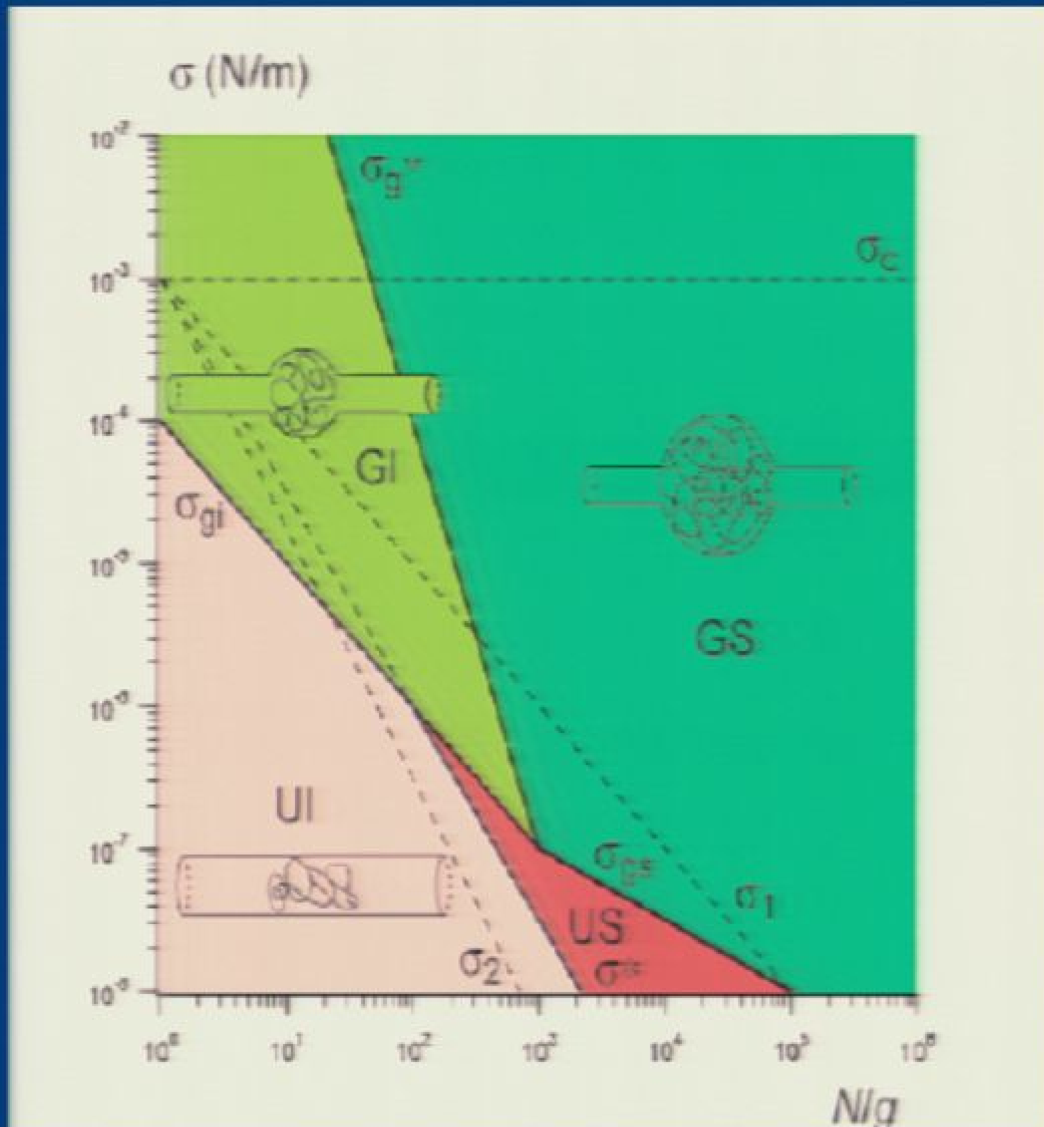
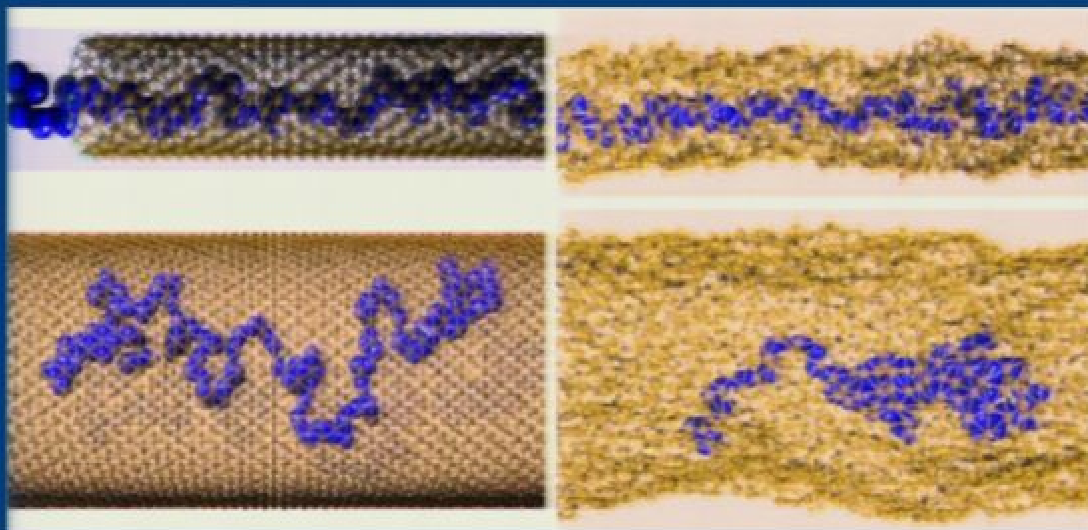
Swollen to globular transition

by Brochard-Wyart, Tanaka, Borghi and de Gennes, Langmuir (2005)



Computer simulation by Avramova and Milchev



Avramova and Milchev, J. Chem. Phys. **124**, 024909 (2006)

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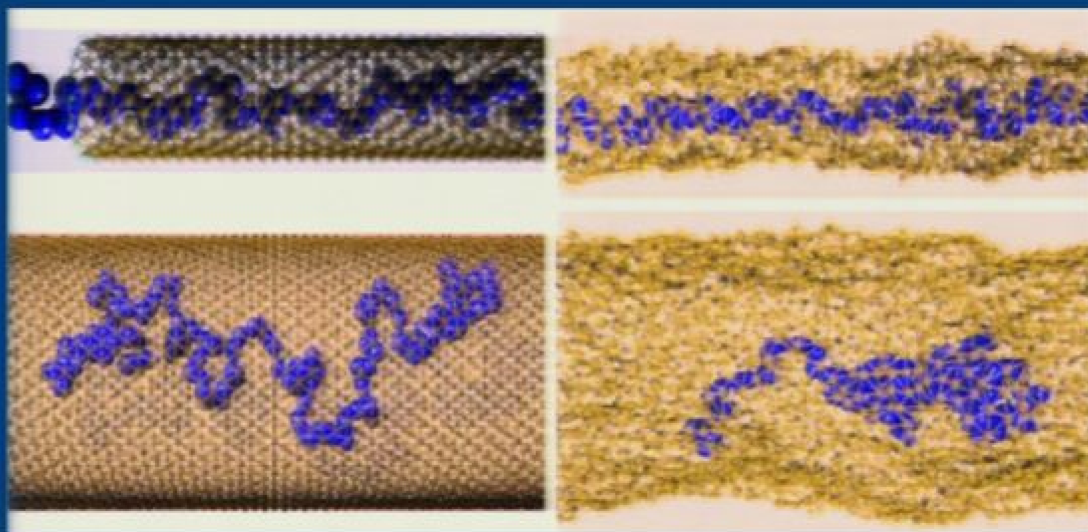

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- Tube must be modeled differently from the theory

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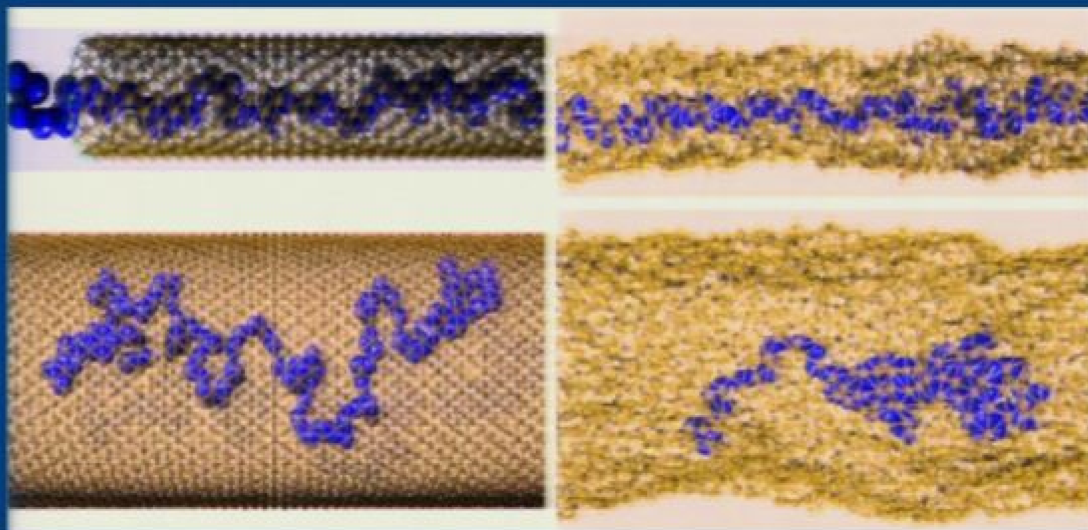

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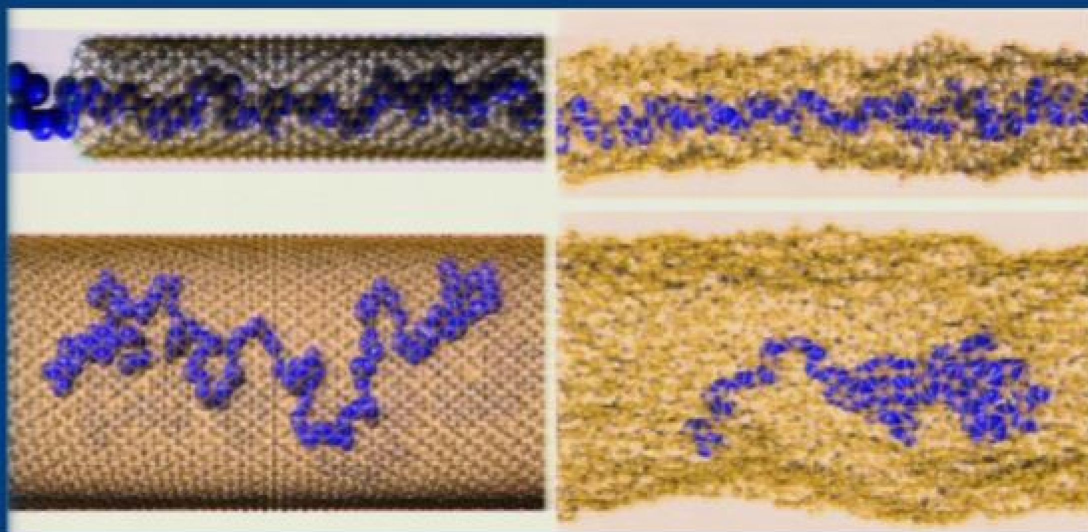

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- Tube must be modeled differently from the theory
- No observations of the structural transition
- Expensive in modeling the tube (a M*M problem)

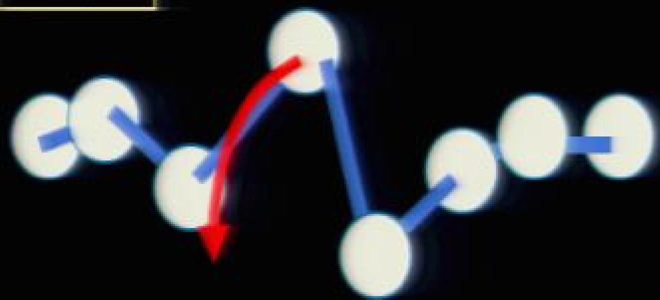
Monte Carlo Simulation of a self-avoiding chain

Step k

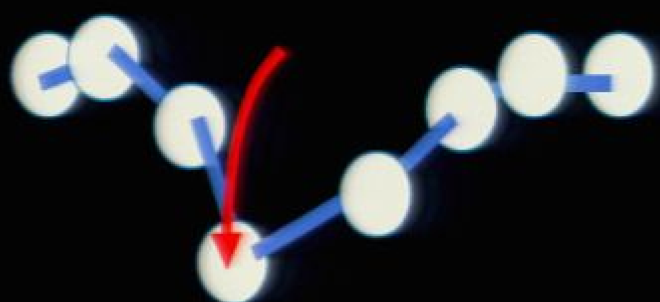
Step k+1

Monte Carlo Simulation of a self-avoiding chain

Step k



Step k+1



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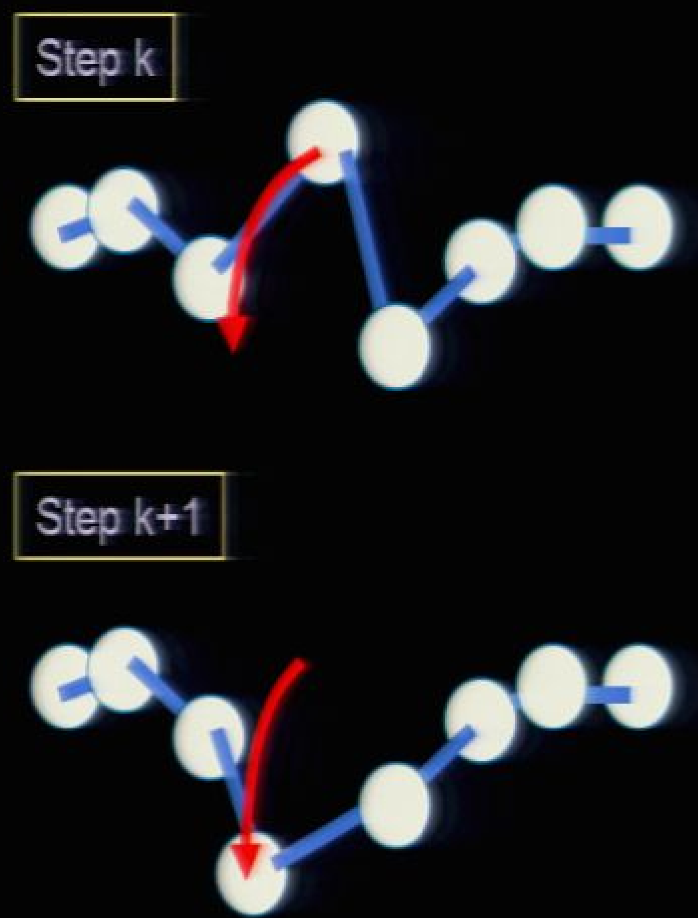

Basic parameters

Bond length a

Total no. of

Monte Carlo Simulation of a self-avoiding chain

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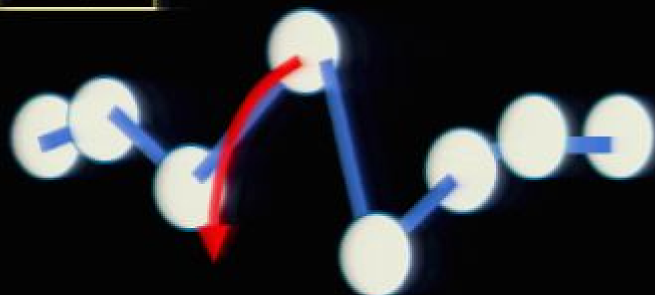

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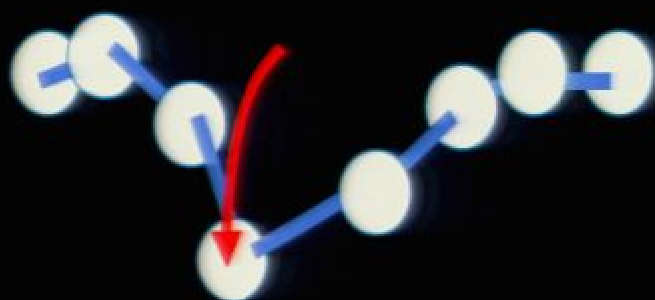

Basic parameters

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Total no. of monomers: N

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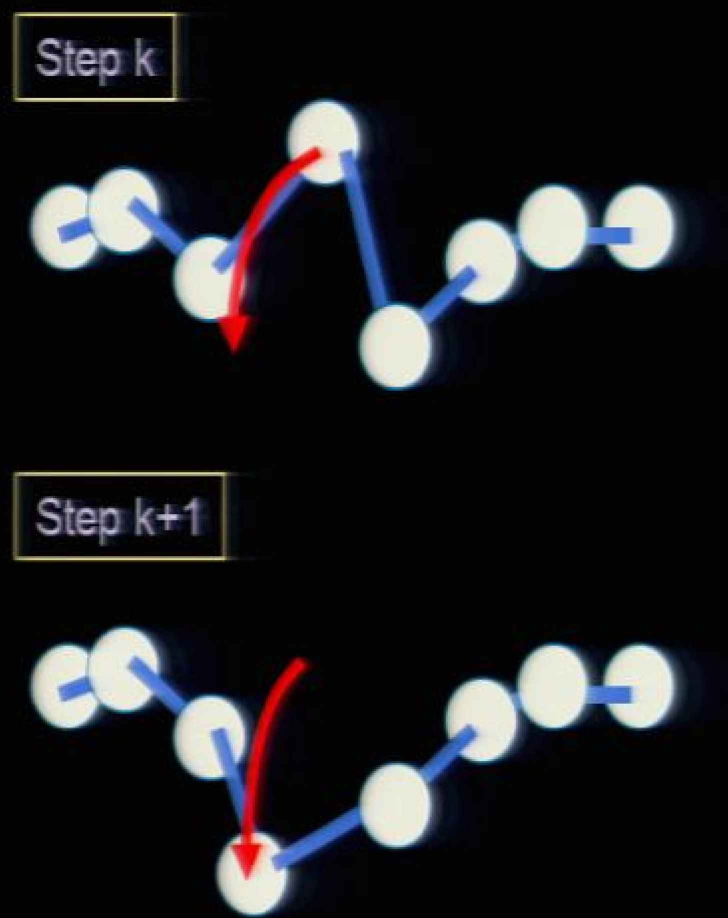

Basic parameters

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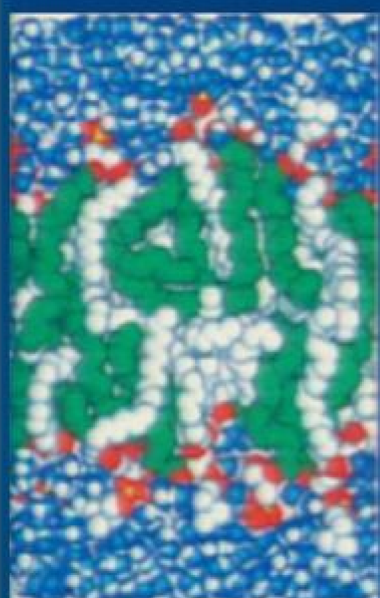
Excluded-volume diameter: D(=a)

Lipid bilayer models

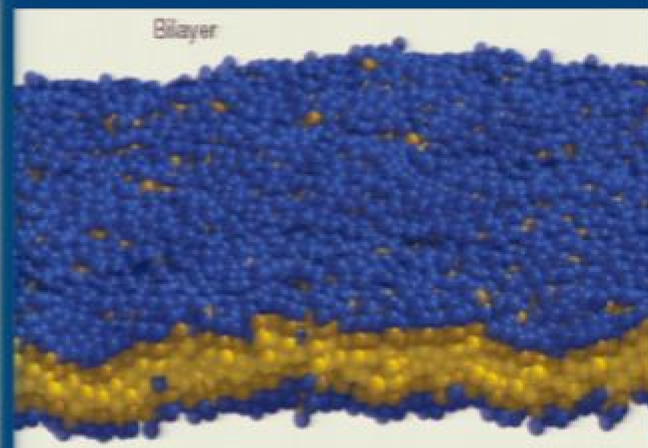
Lipid bilayer models

- All-atom model



Lipid bilayer models

- Coarse grained



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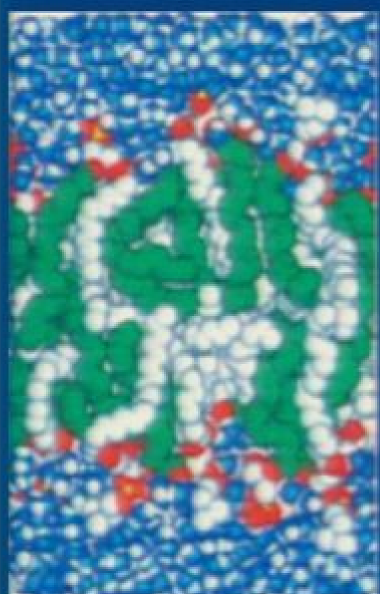

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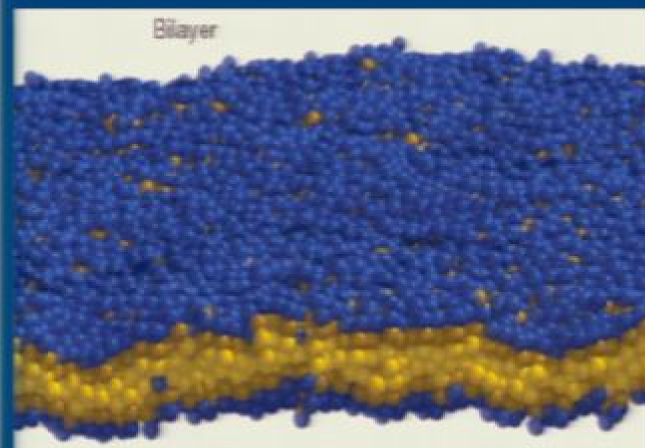
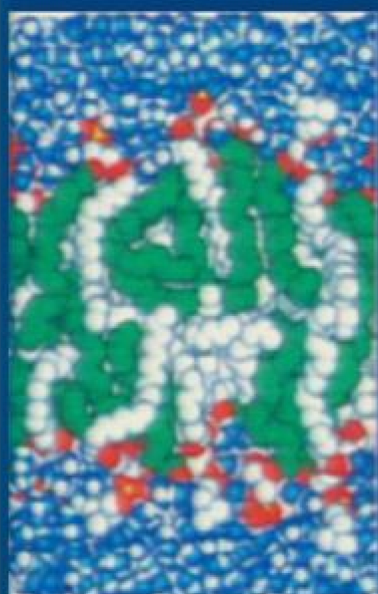
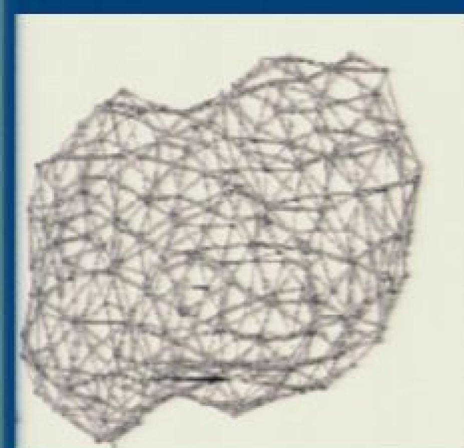


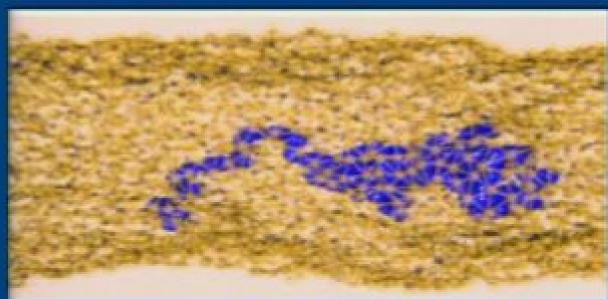
- All-atom model



- Elastic sheet

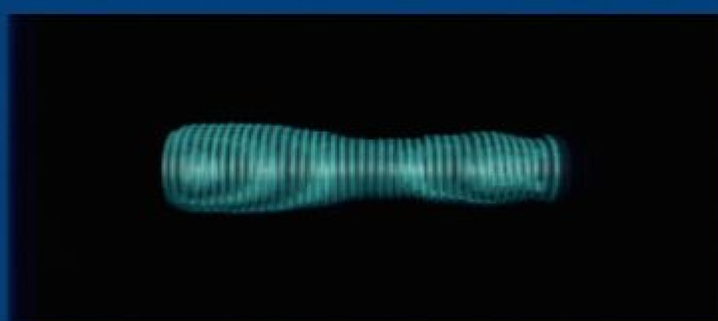


Representation of a tube membrane



Elastic sheet techniques

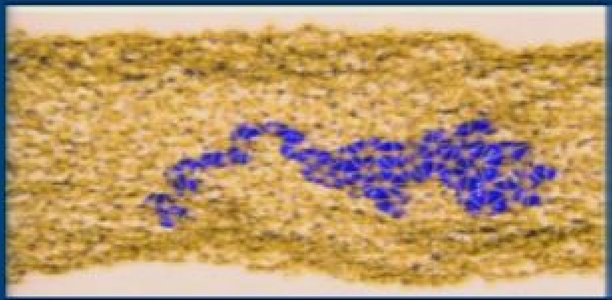
- M^2 nodes needed
- Complex to maintain a tube



Our technique

- Only M nodes needed
- Use Helfrich model directly

Representation of a tube membrane



Elastic sheet techniques

- M^2 nodes needed
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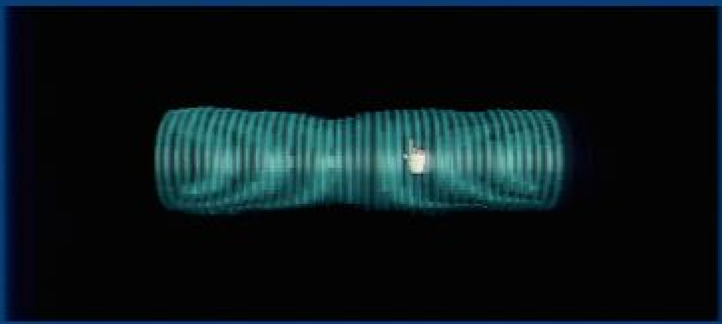

Our technique

- Only M nodes needed
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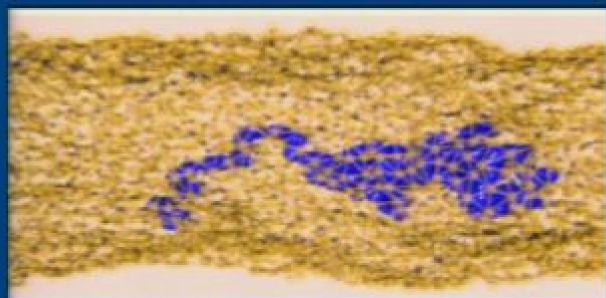
Representation of a tube membrane



Elastic sheet techniques

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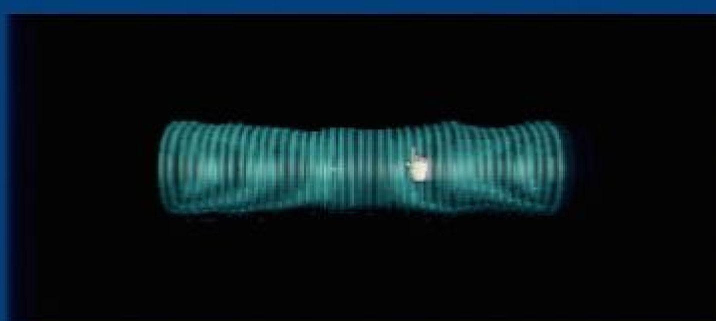
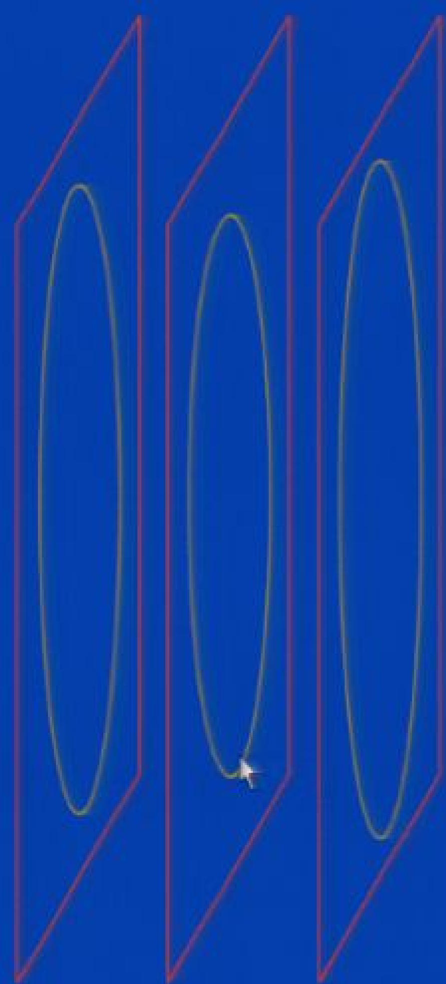


Our technique

- Only M nodes needed
- Use Helfrich model directly

Helfrich energy for a soft tube



Radius: R_{i-1} R_i R_{i+1}

- Geometrical:

  area: $\Delta A(R_{i-1},R_i,R_{i+1})$

  inverse curvatures: $r_1(R_{i-1},R_i,R_{i+1})$
  $r_2(R_{i-1},R_i,R_{i+1})$

- E_i
  $= \Delta A\,[\sigma + (\kappa/2)\,(1/r_1+1/r_2)^2\,]$
  = function of R_{i-1},R_i,R_{i+1} with two physical parameters κ and σ

- $E = \sum_{i=1}^{M} E_i$

Monte Carlo simulation for a tube membrane confining a polymer

- Select a random i
- Move R_i^2
- Calculate energy difference between the new and old systems
- Evaluate the acceptability of the new configuration using

$$P = \exp[-\beta \Delta E]$$

(Metropolis Monte Carlo)

- Move the polymer inside
- Go back to the first step

Always check to see if the polymer is confined inside

Parameters in the model

Parameters in the model

- N, a (polymer)
- κ, σ (membrane)

Parameters in the model

- N, a (polymer)
- κ, σ (membrane)
- β (inverse temperature introduced in the Monte Carlo procedure)

Parameters in the model

- N, a (polymer)
- κ, σ (membrane)
- β (inverse temperature introduced in the Monte Carlo procedure)

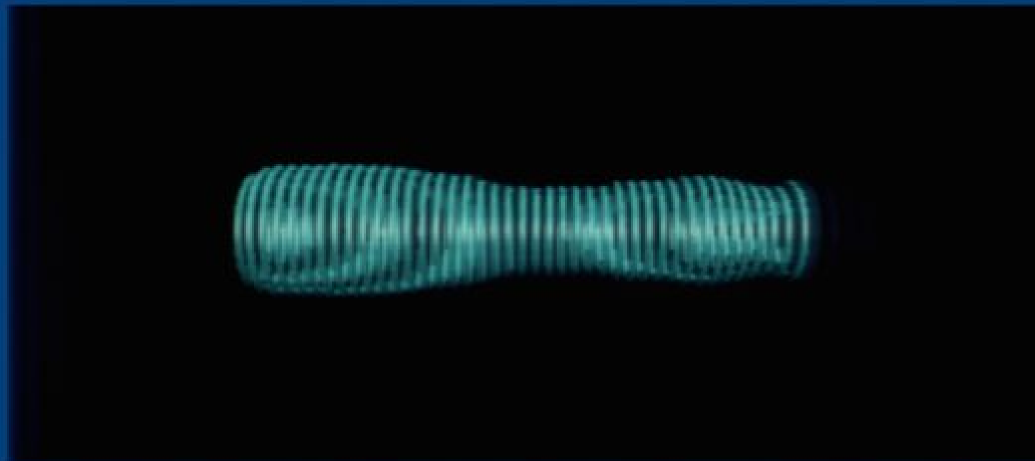
Reduced Parameters in the model

Parameters in the model

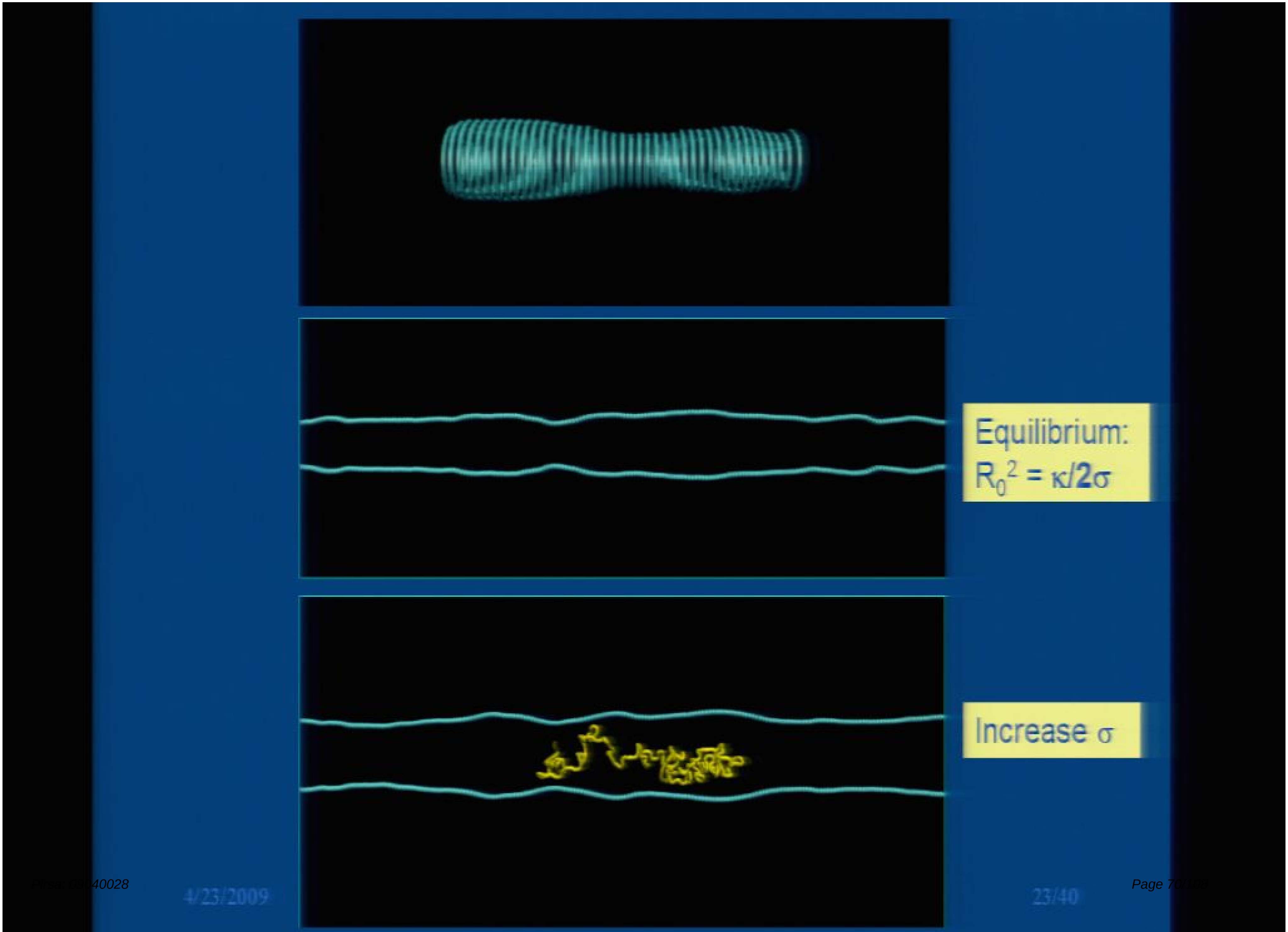
- N, a (polymer)
- κ, σ (membrane)
- β (inverse temperature introduced in the Monte Carlo procedure)

Reduced Parameters in the model

- N (polymer)
- $\beta\sigma a^2$
- $\beta\kappa$ (we FIX $\beta\kappa$ in the remainder of this talk)

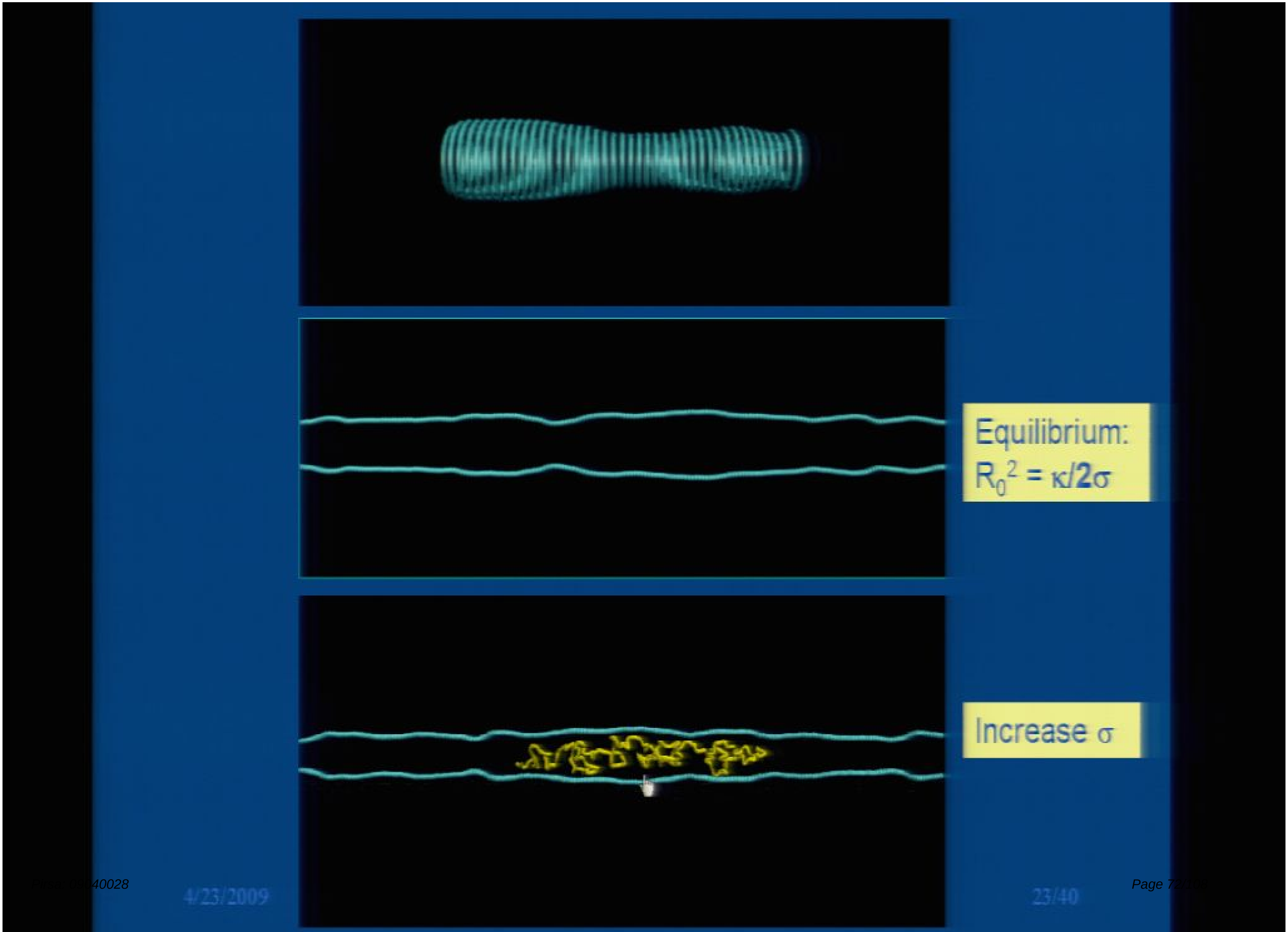


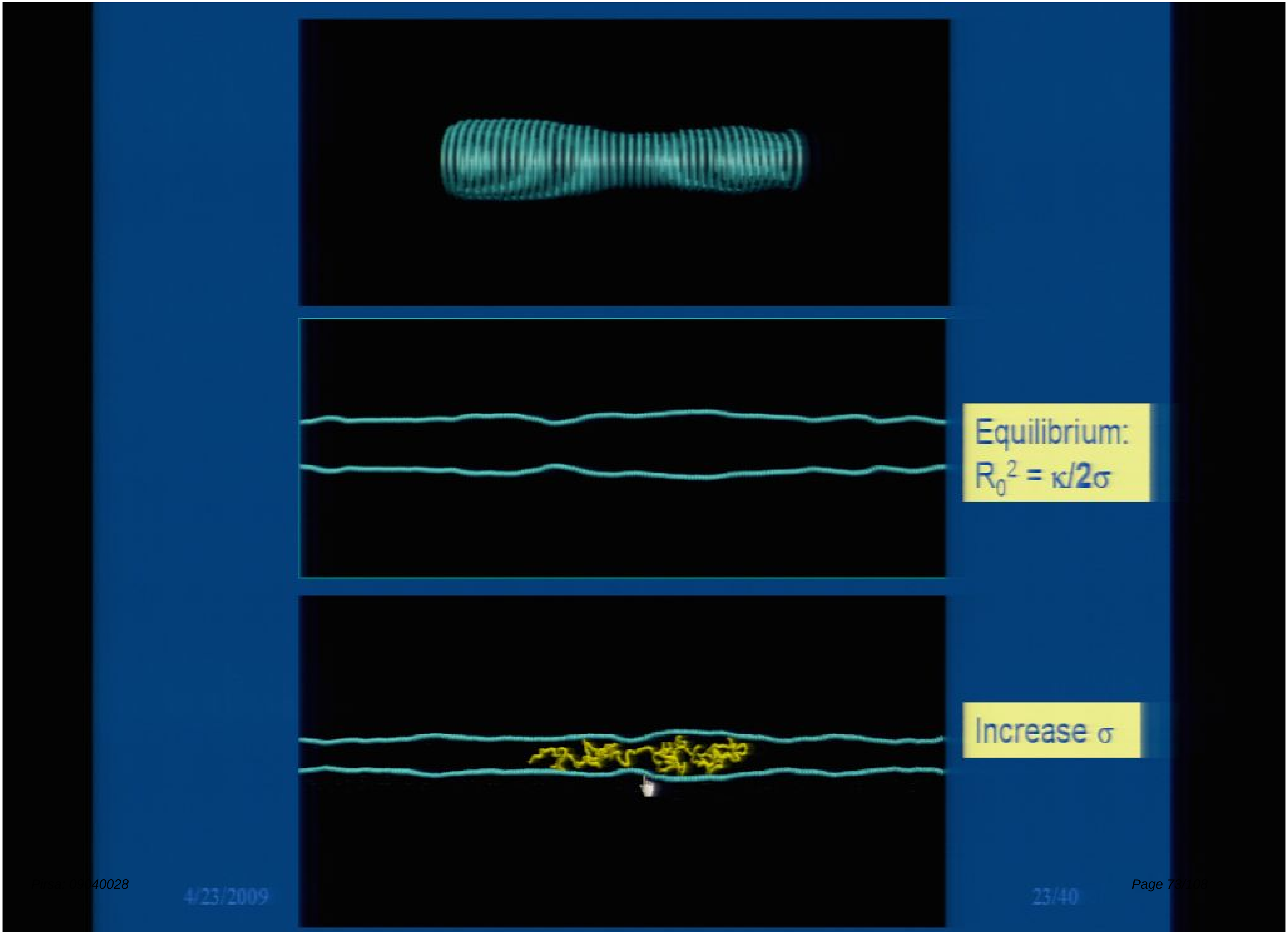

Equilibrium:
$R_0^2 = \kappa/2\sigma$
4/23/2009
PI 4 corners
23/40

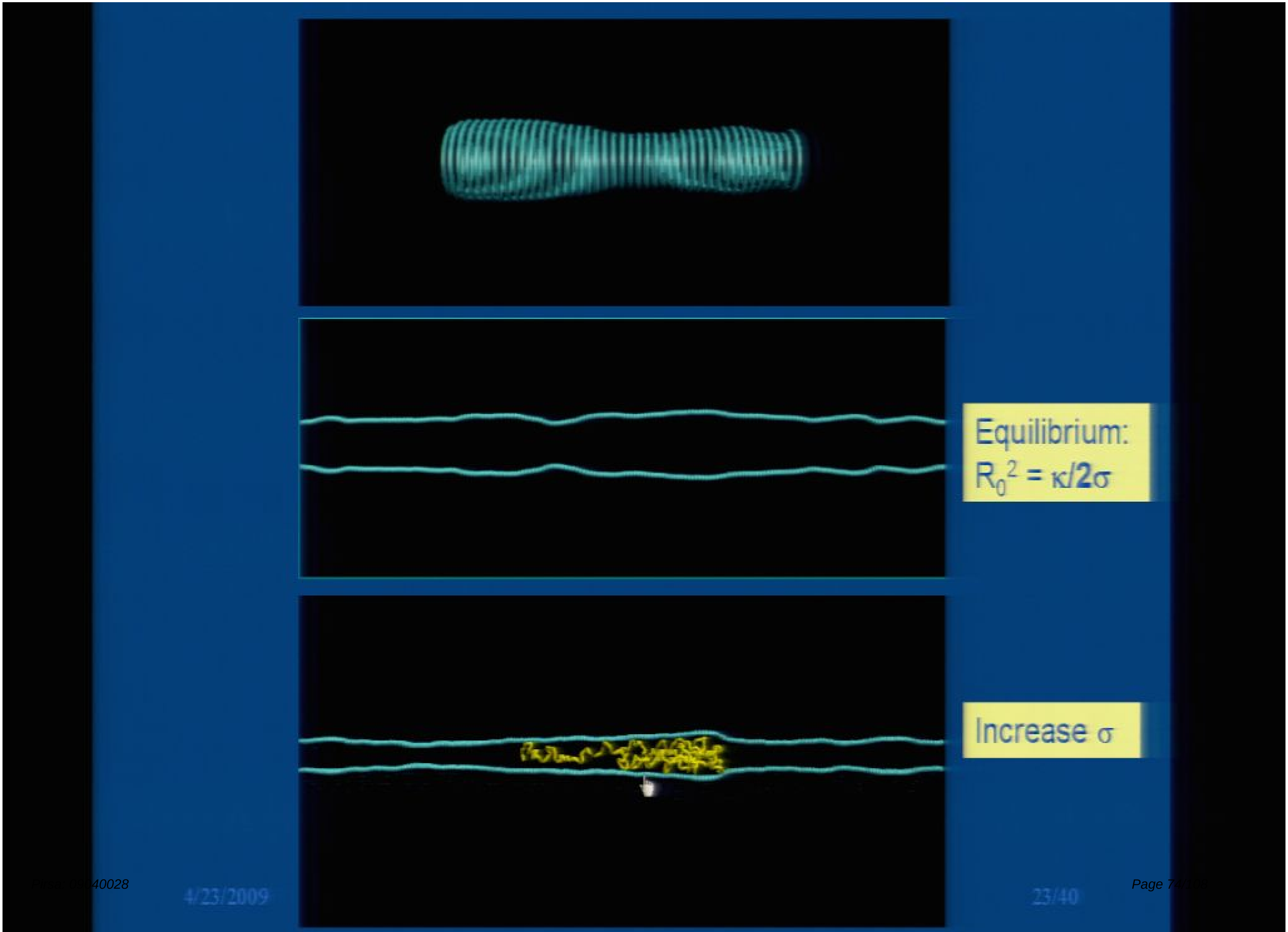


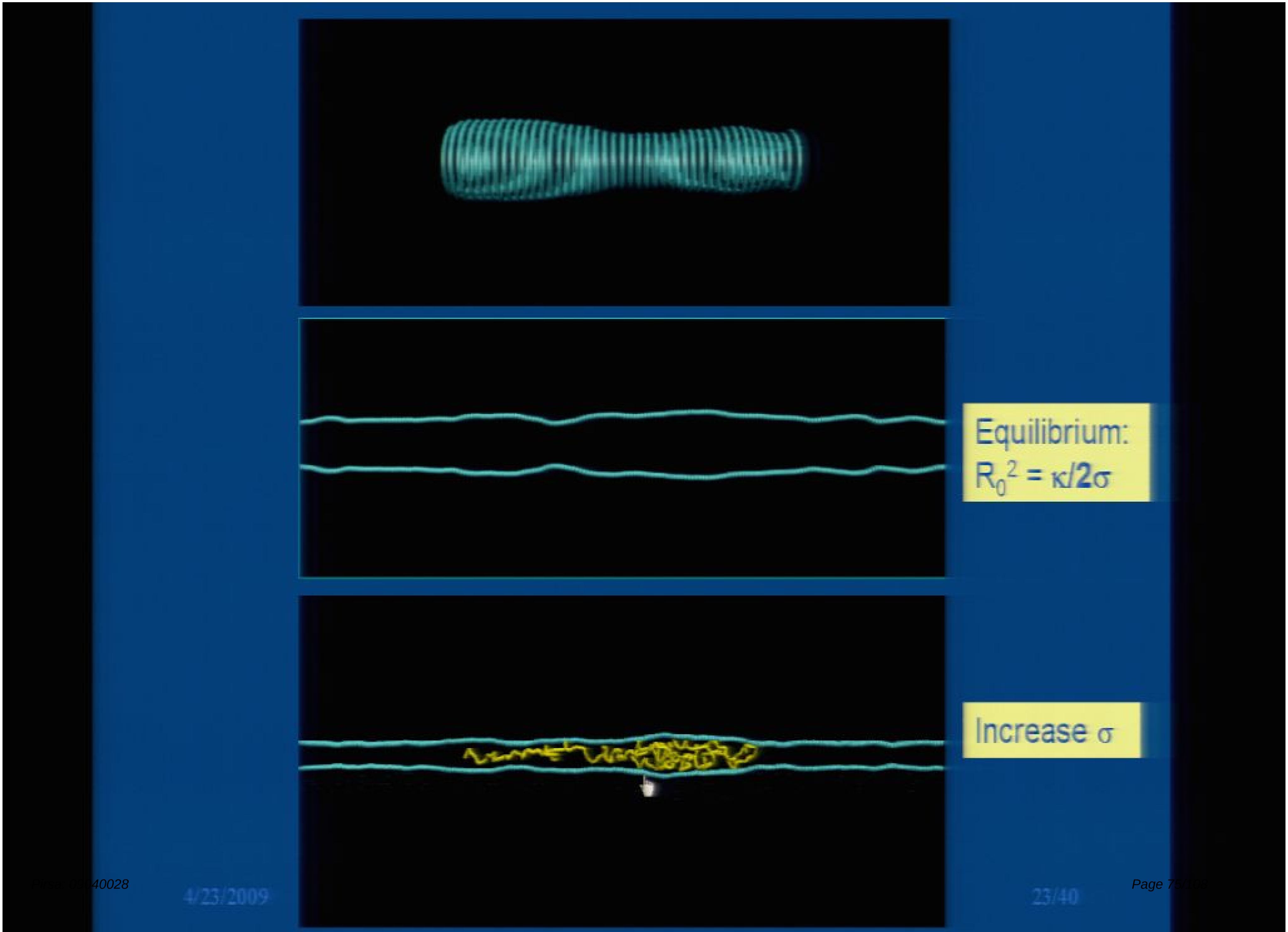
Equilibrium:
$R_0^2 = \kappa/2\sigma$
Increase σ
4/23/2009
23/40


Equilibrium:
$R_0^2 = \kappa/2\sigma$
Increase σ
4/23/2009
23/40


Equilibrium:
$R_0^2 = \kappa/2\sigma$
Increase σ
4/23/2009
23/40


Equilibrium:
$R_0^2 = \kappa/2\sigma$
Increase σ
4/23/2009
23/40


Equilibrium:
$R_0^2 = \kappa/2\sigma$
Increase σ
4/23/2009
23/40


Equilibrium:
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Increase σ
4/23/2009
23/40

Equilibrium:
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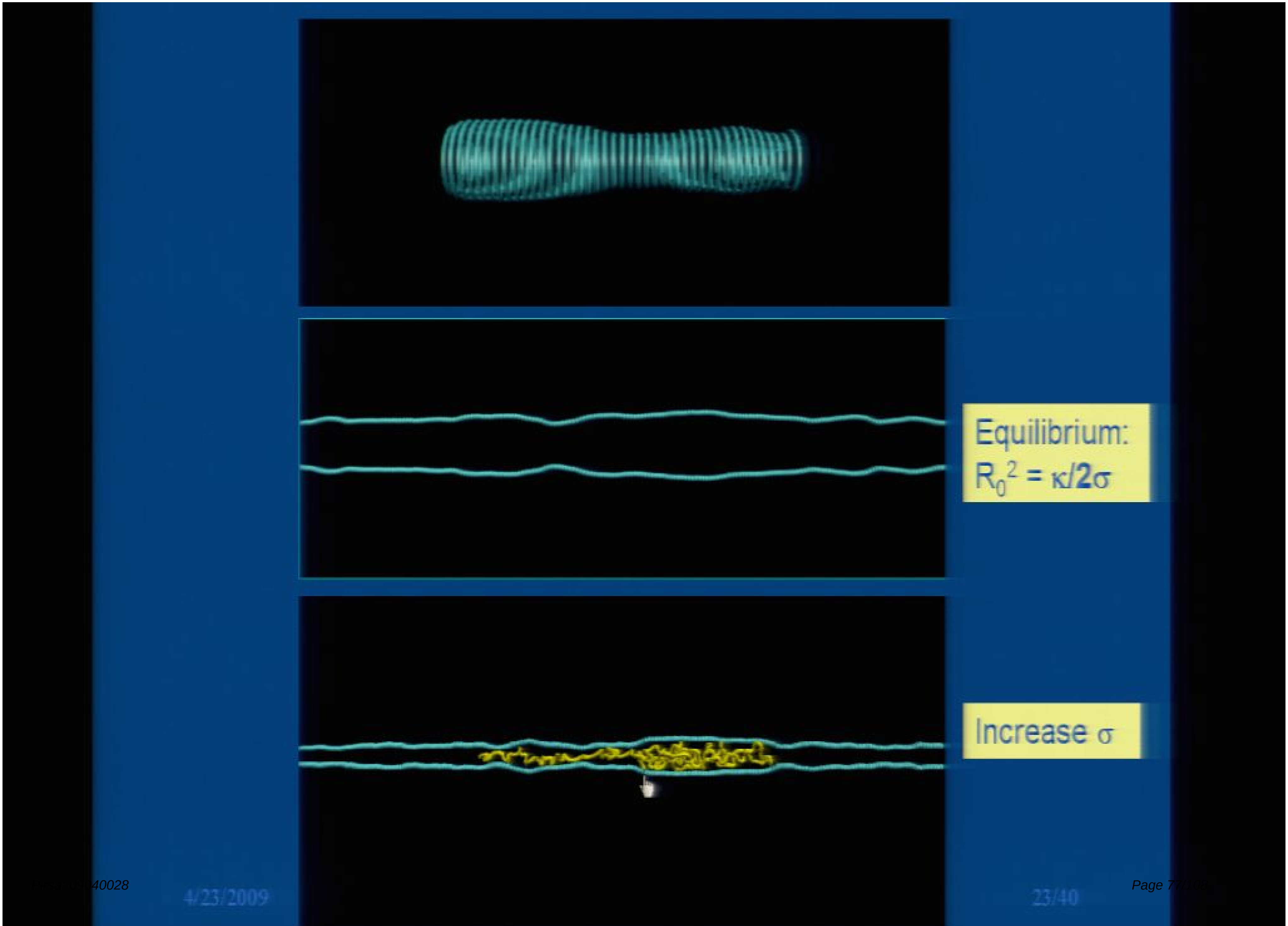
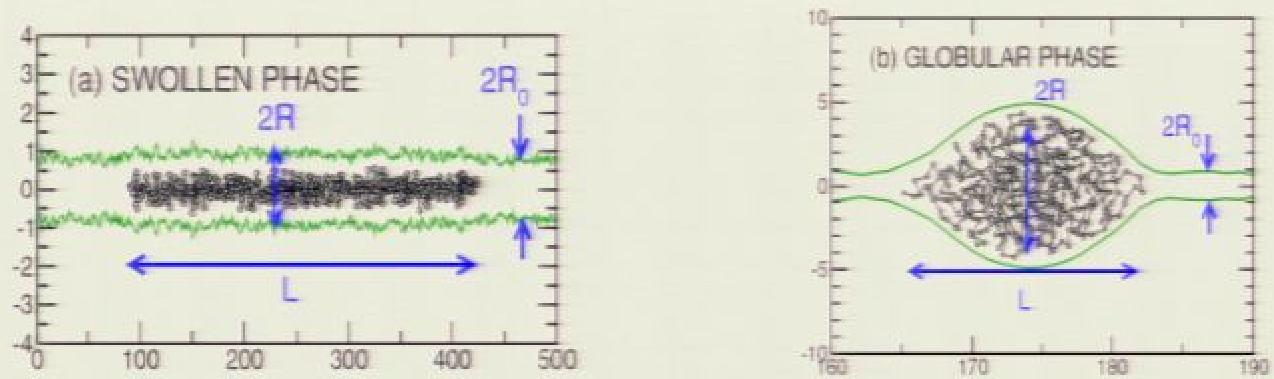
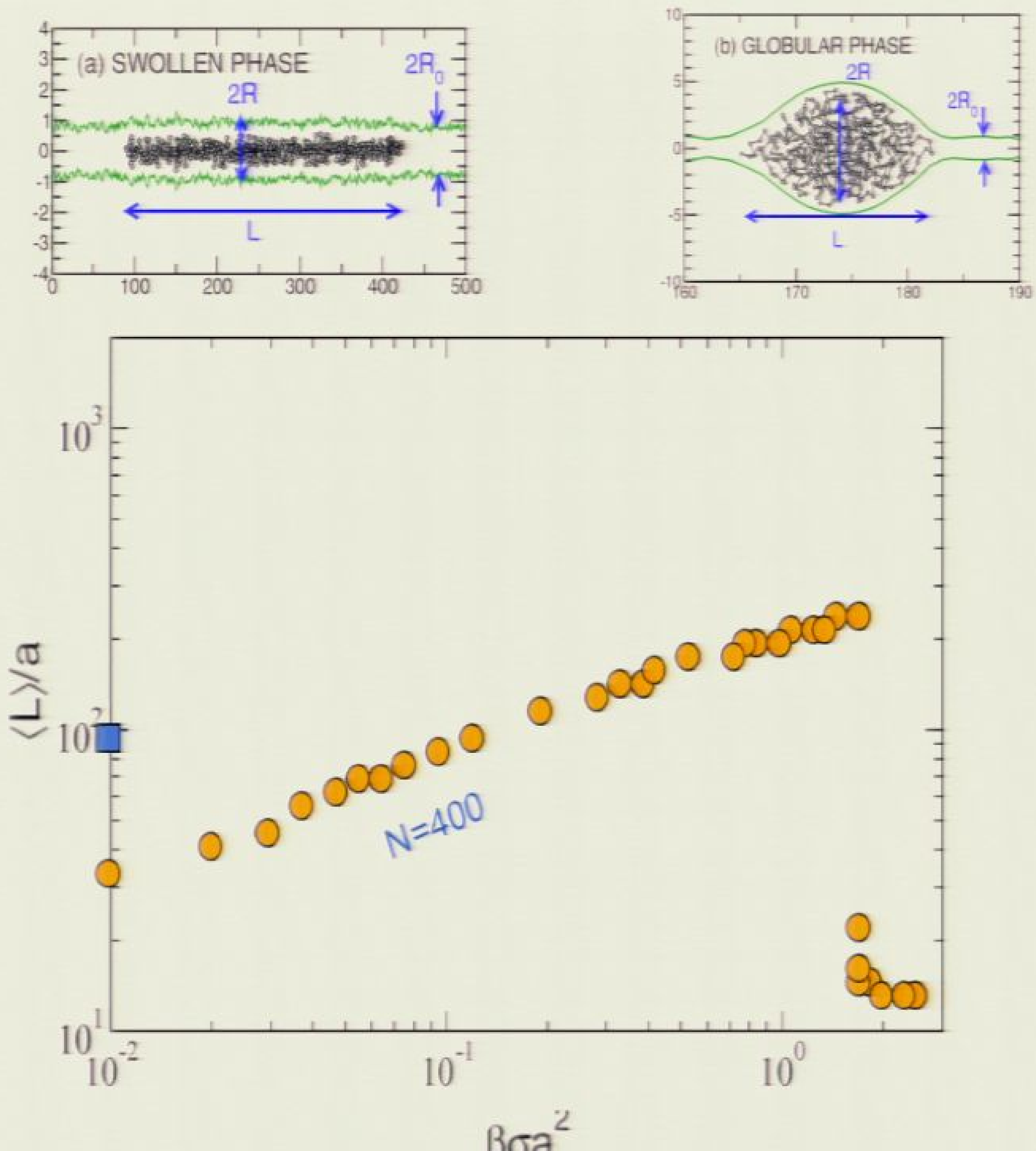
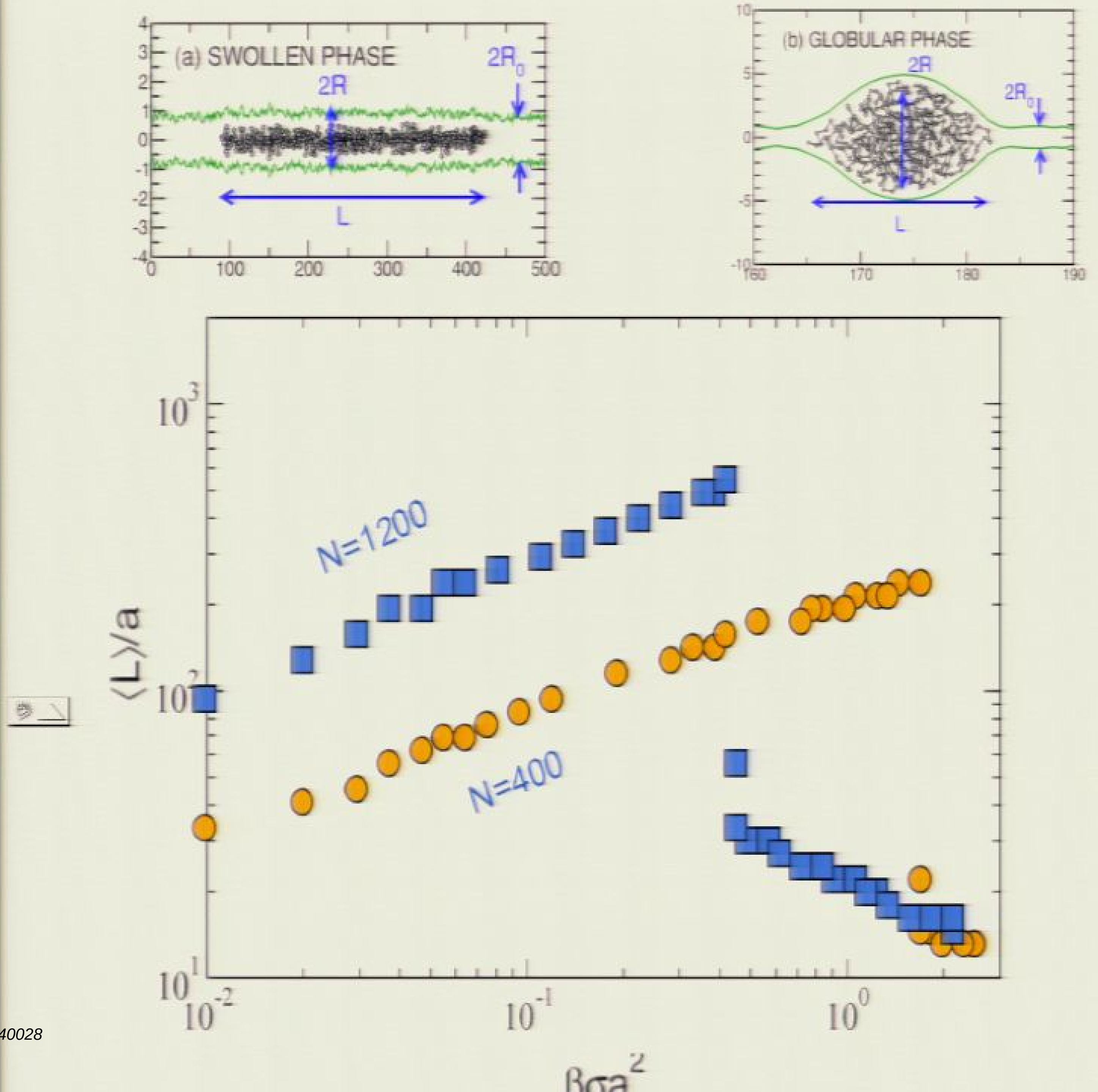
23/40

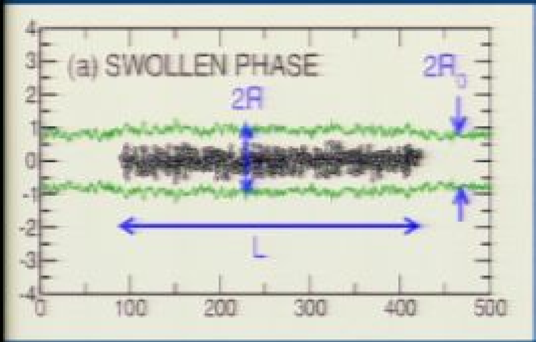

Equilibrium:
$R_0^2 = \kappa/2\sigma$
Increase σ
4/23/2009
23/40

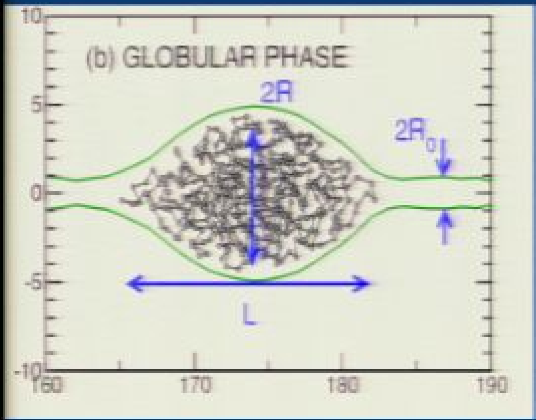

(a) SWOLLEN PHASE
2R
$2R_0$
L
(b) GLOBULAR PHASE
2R
$2R_0$
L


(a) SWOLLEN PHASE
2R
2R0
L
(b) GLOBULAR PHASE
2R
2R0
L
N=400
⟨L⟩/a
βσa²

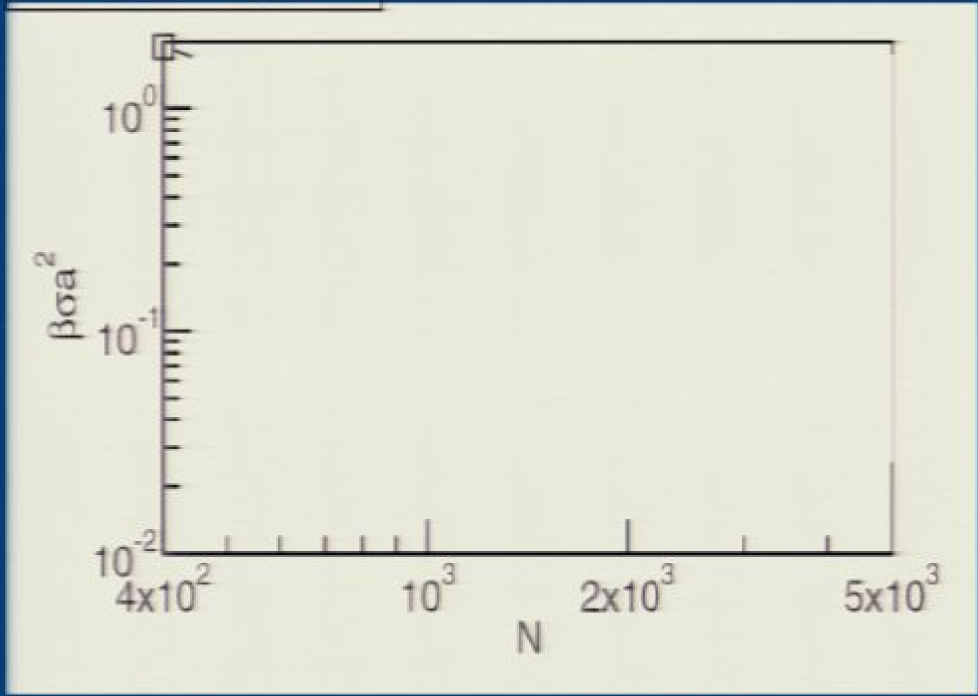


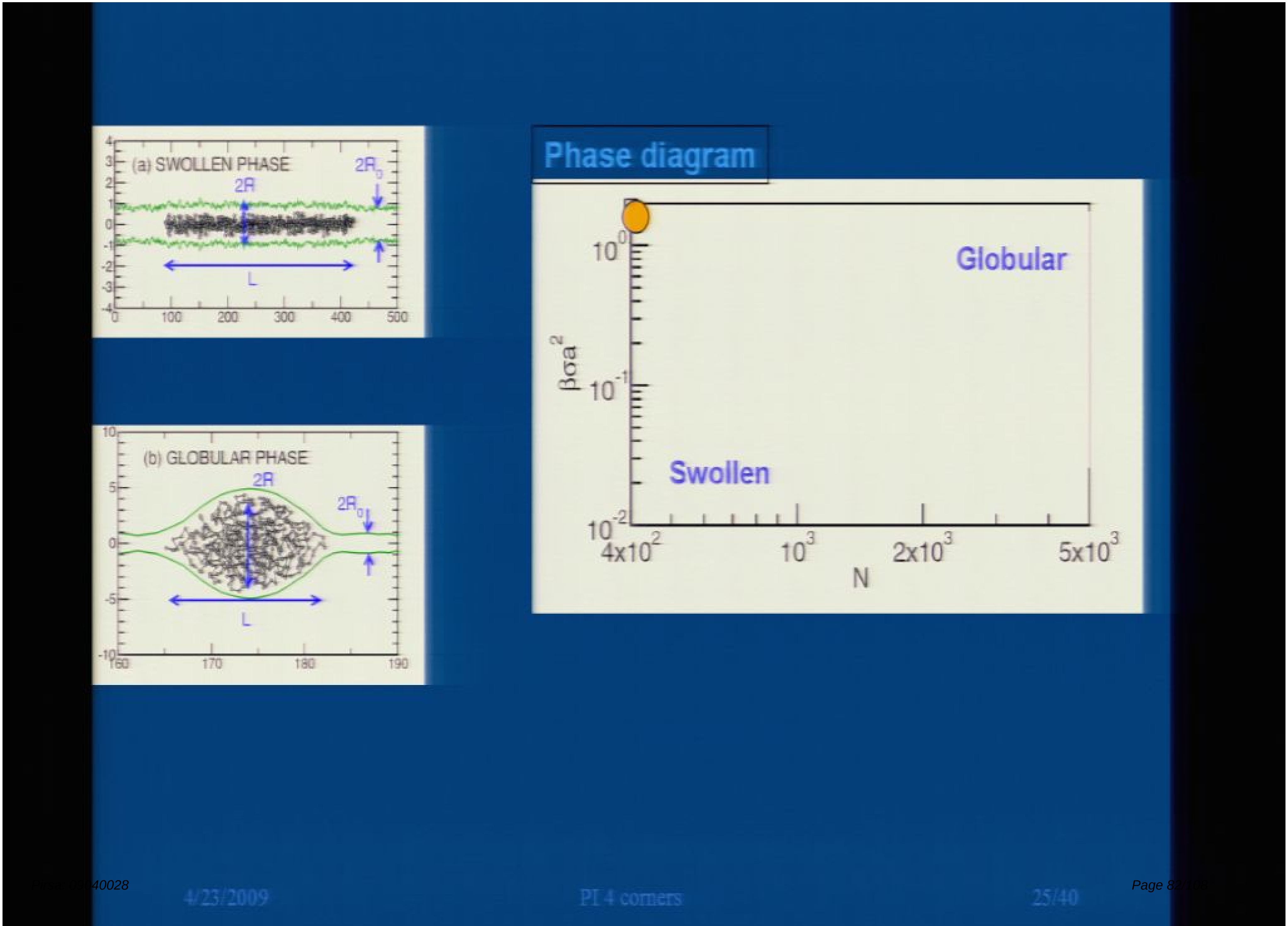
(a) SWOLLEN PHASE
2R
2R0
L
(b) GLOBULAR PHASE
2R
2R0
L
N=1200
N=400
⟨L⟩/a
βσa²

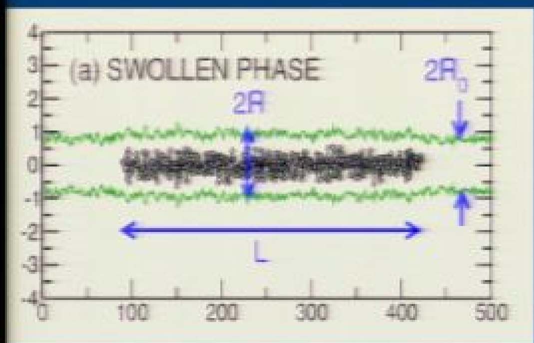


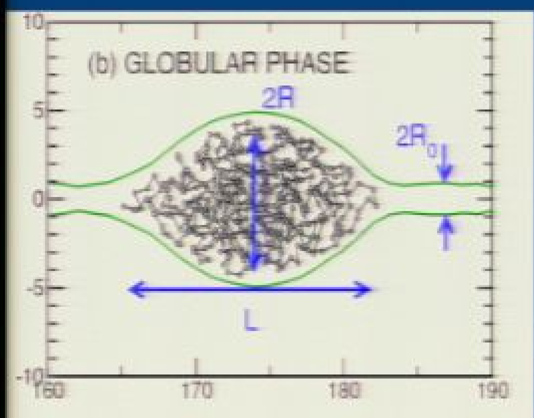


Phase diagram

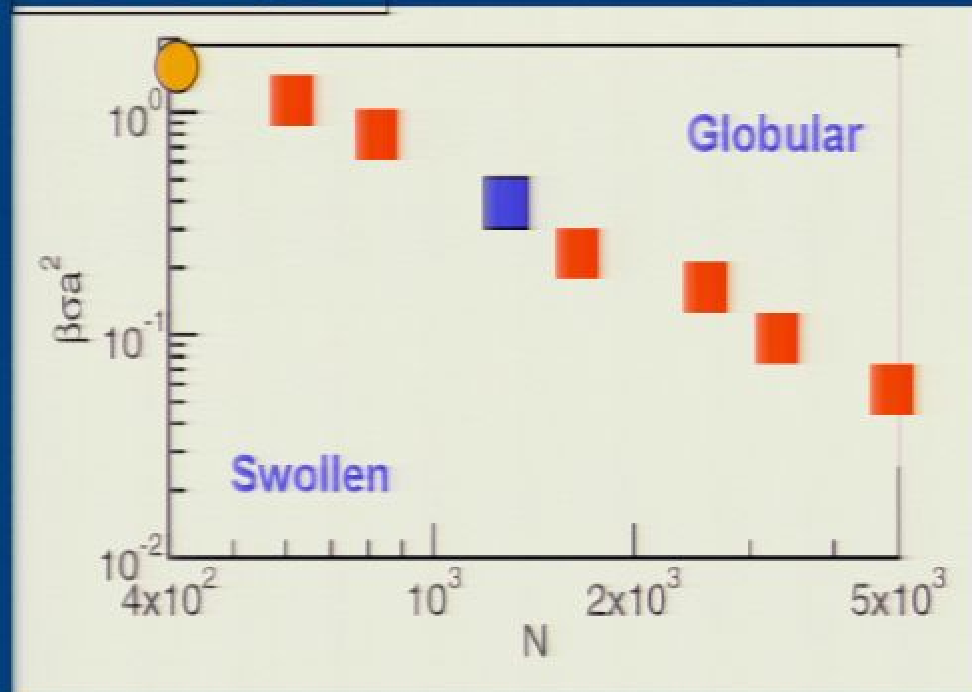



Phase diagram
(a) SWOLLEN PHASE
2R
$2R_0$
L
(b) GLOBULAR PHASE
2R
$2R_0$
L
Globular
Swollen
$\beta\sigma a^2$
10^0
10^{-1}
10^{-2}
4×10^2
10^3
2×10^3
5×10^3
N
4/23/2009
PI 4 corners
25/40

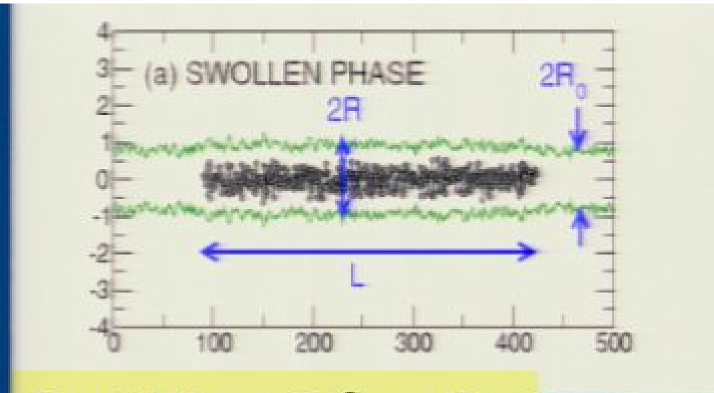




Phase diagram

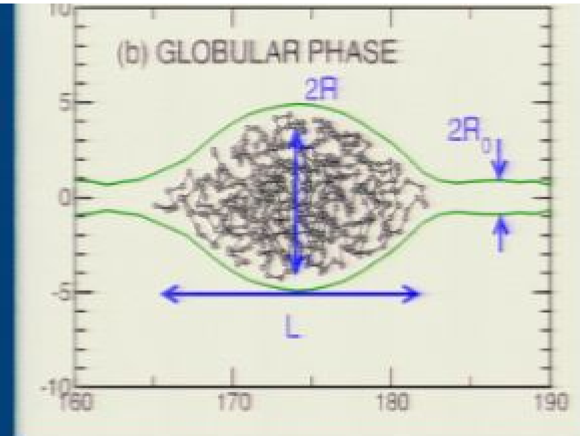


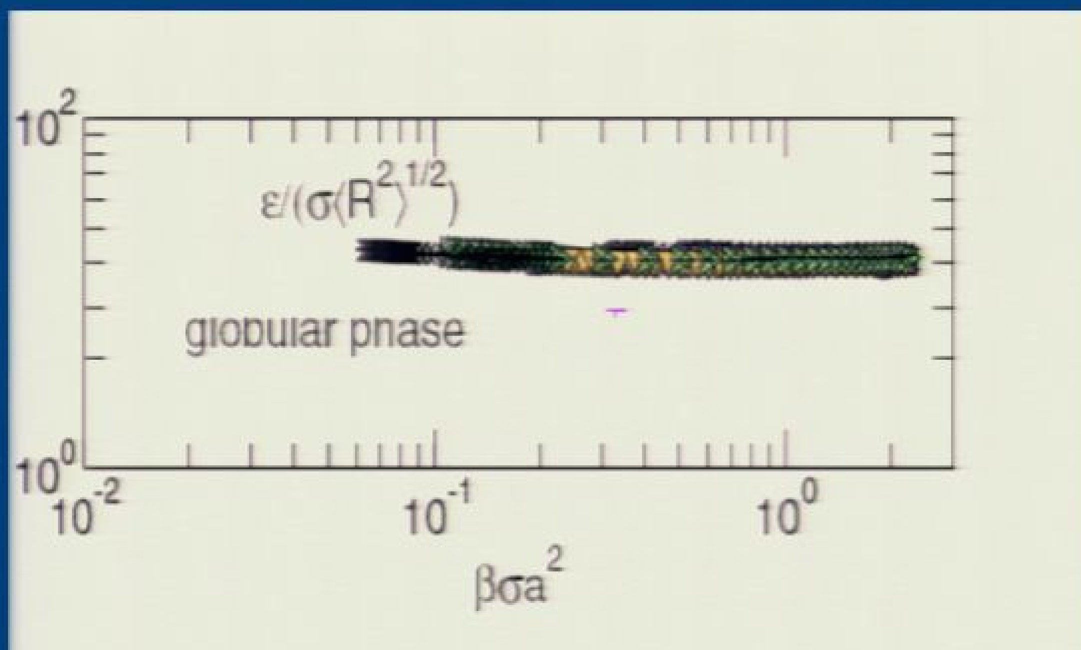
Properties of the swollen phase



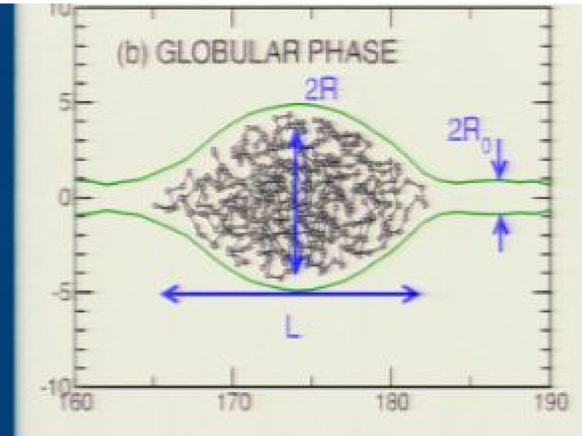
Equilibrium: $R_0^2 = \kappa/2\sigma$

Properties of the globular phase





Properties of the globular phase

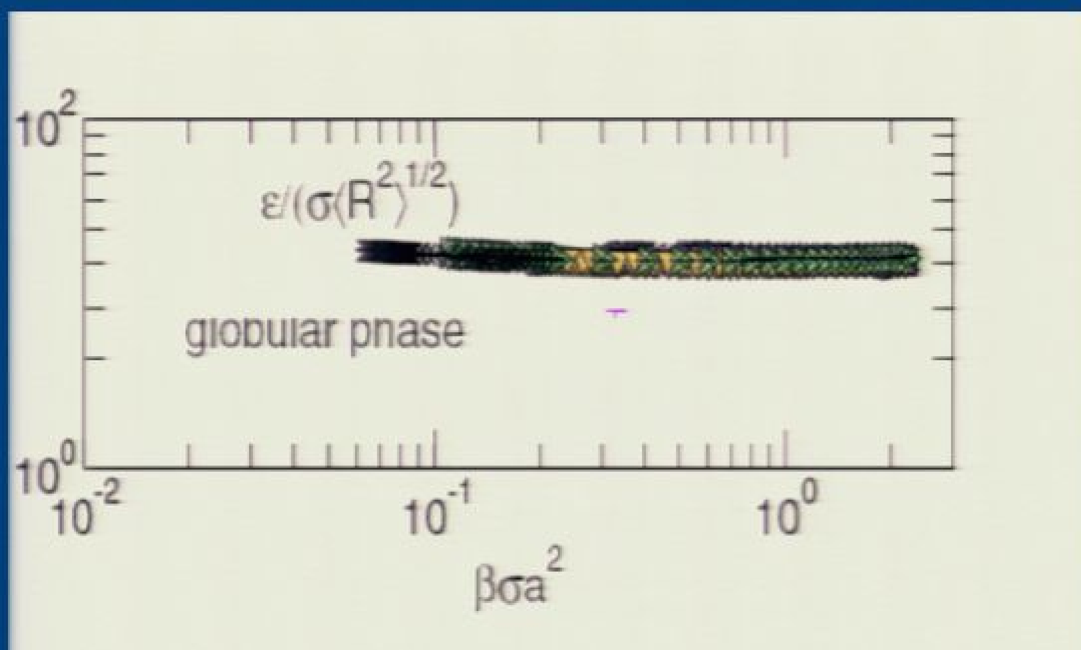


Helfrich energy = $\Delta A\,[\sigma + (\kappa/2)\,(1/r_1+1/r_2)^2\,]$

$\sim \Delta A\,\sigma + \ldots$

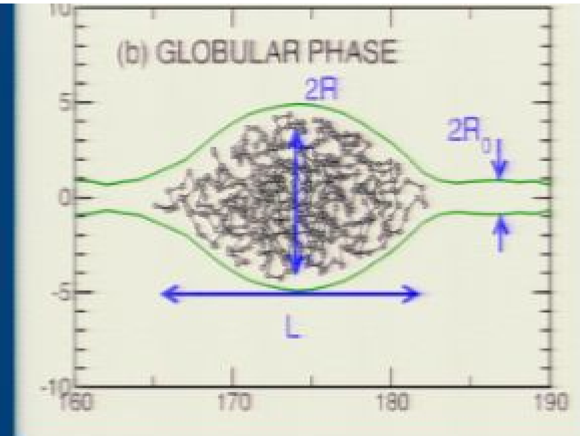
Total energy = $2\pi \langle R^2\rangle^{1/2} L\,\sigma$

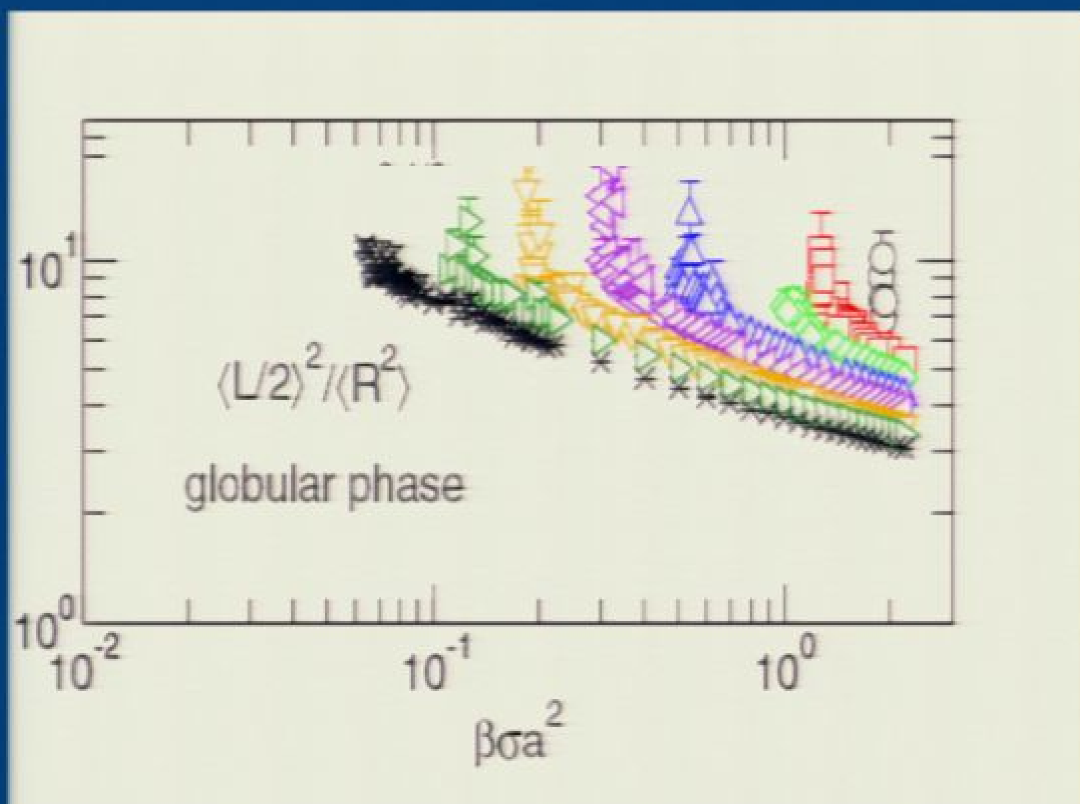
Total energy/L = $\varepsilon = 2\pi \langle R^2\rangle^{1/2}\,\sigma$



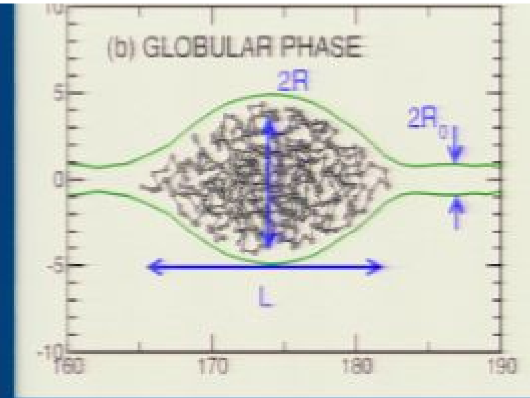
Properties of the globular phase

Scaling theory: L ~ R



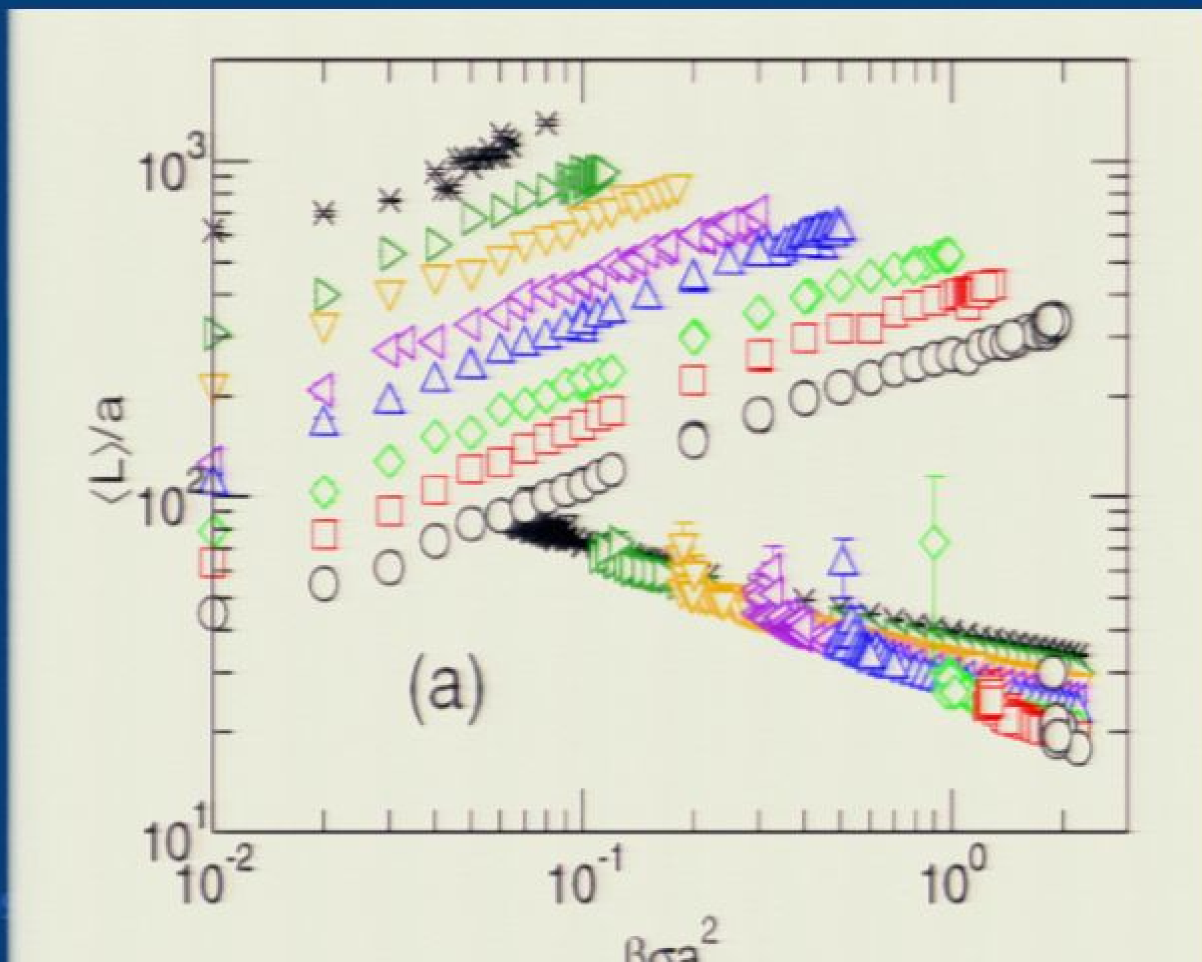


Properties of the globular phase



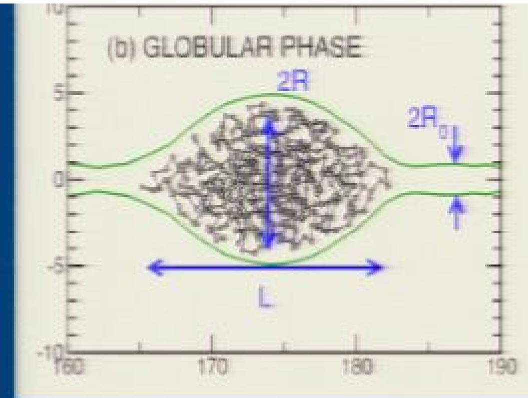
$$\langle L \rangle = \text{Constant}\ N^{\alpha}\sigma^{-\beta}$$

- Scaling theory: a=2/5, b=1/5



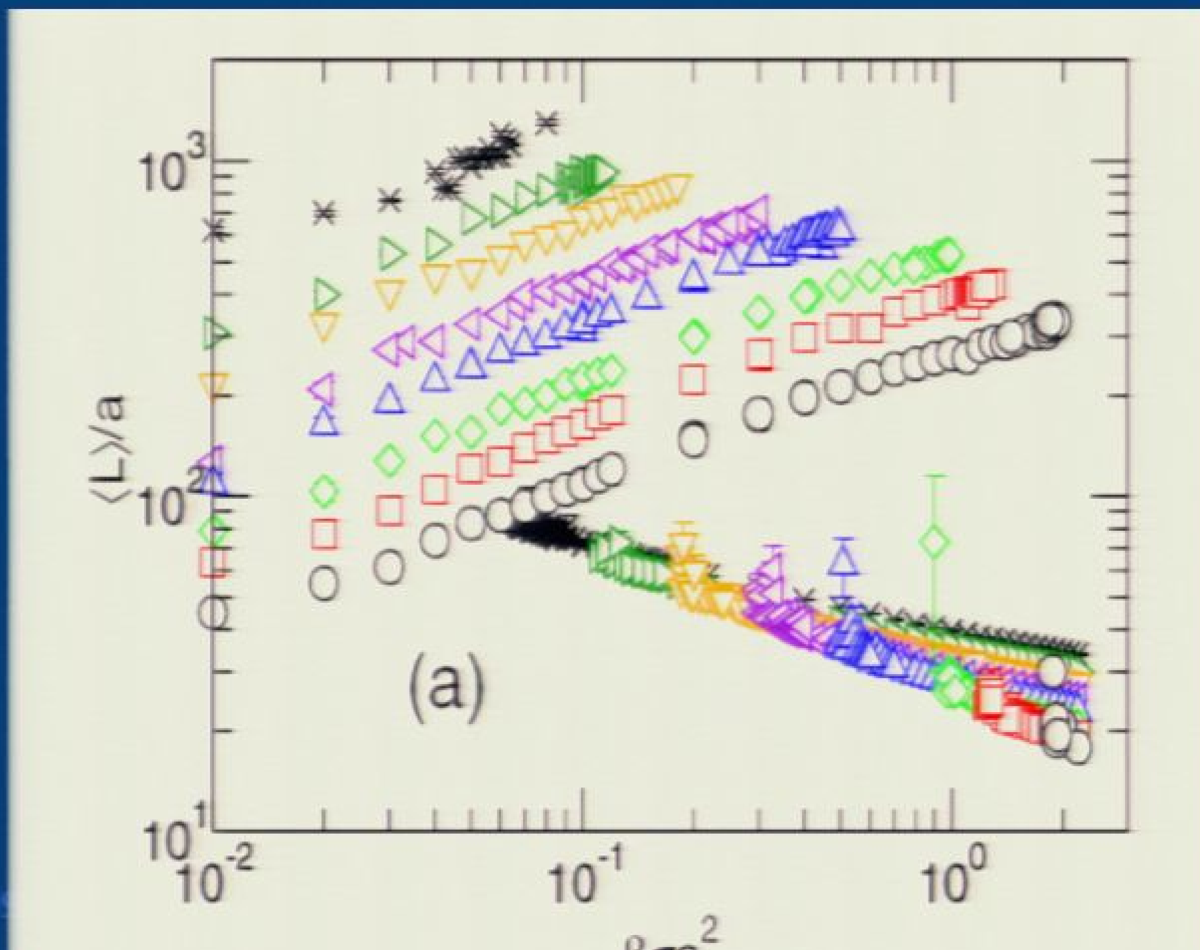

TOPIC 2:
Nanospheres
attracted to a flat
membrane
4/23/2009
PI 4 corners
31/40

Properties of the globular phase



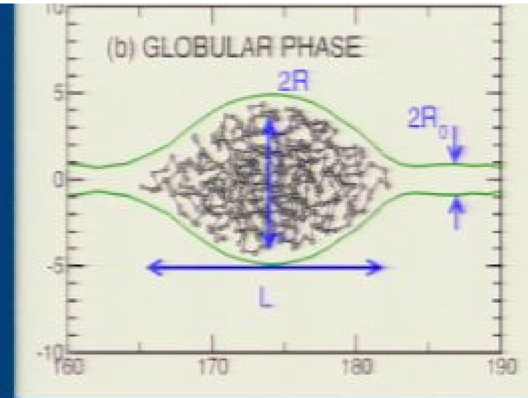
$$\langle L\rangle = \text{Constant } N^{\alpha}\sigma^{-\beta}$$

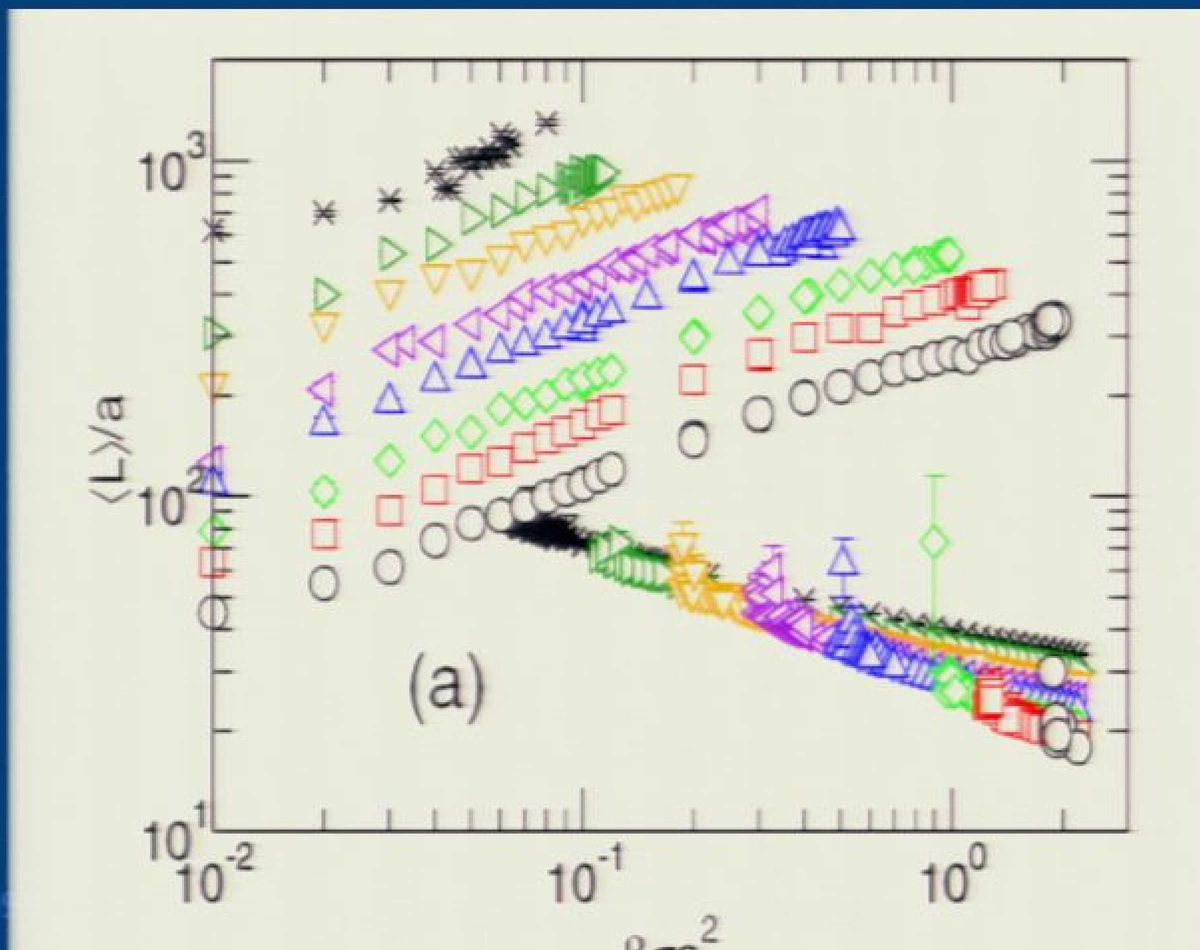
- Scaling theory: a=2/5, b=1/5
- Simulation: much stronger dependence

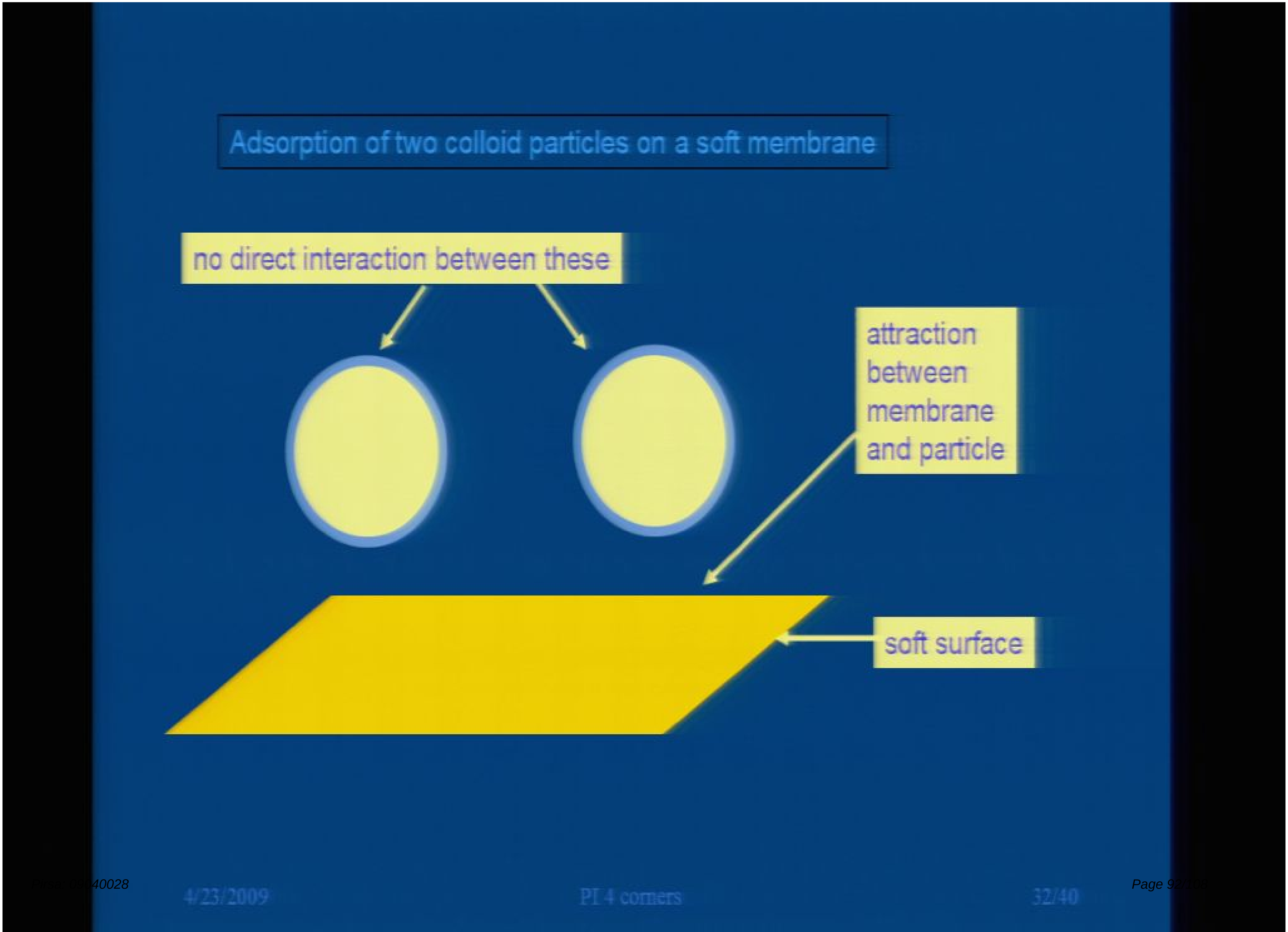


Properties of the globular phase

$$\langle L \rangle = \text{Constant}\ N^{\alpha} \sigma^{-\beta}$$





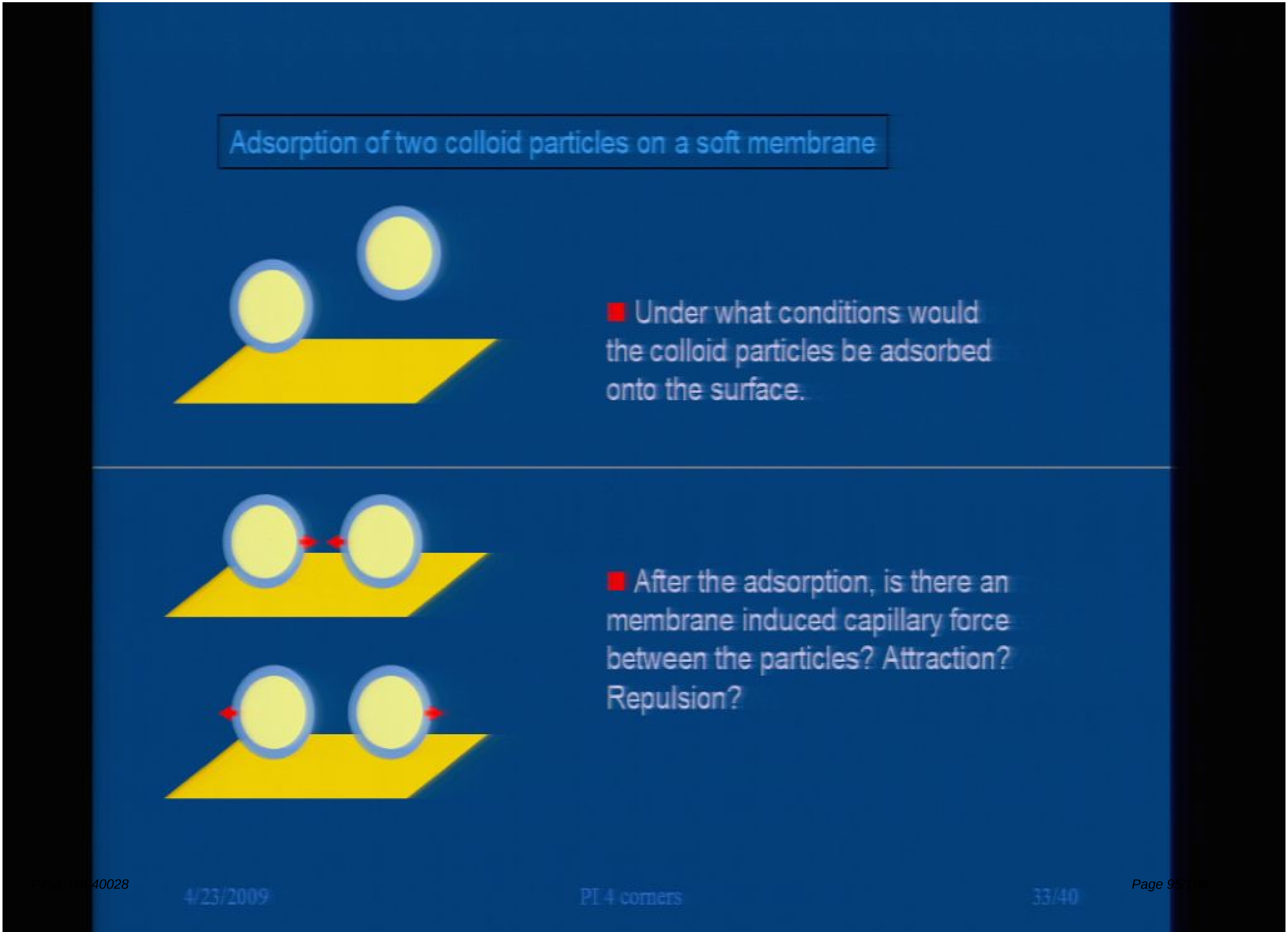

Adsorption of two colloid particles on a soft membrane
no direct interaction between these
attraction between membrane and particle
soft surface
4/23/2009
PI 4 corners
32/40

Adsorption of two colloid particles on a soft membrane

- Under what conditions would the colloid particles be adsorbed onto the surface.

Adsorption of two colloid particles on a soft membrane

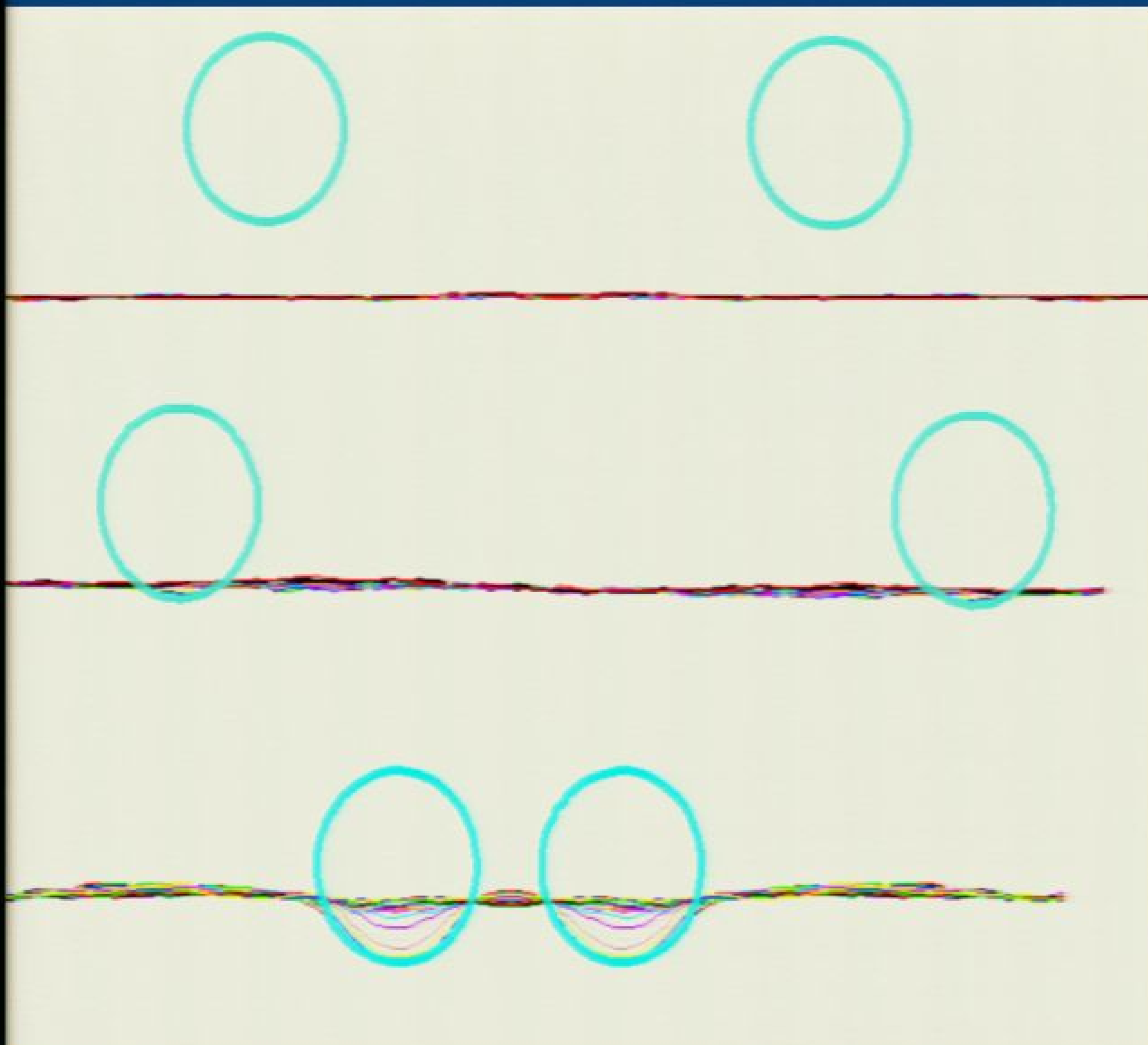
- Under what conditions would the colloid particles be adsorbed onto the surface.



Adsorption of two colloid particles on a soft membrane
Under what conditions would the colloid particles be adsorbed onto the surface.
After the adsorption, is there an membrane induced capillary force between the particles? Attraction? Repulsion?
4/23/2009
PI 4 corners
33/40

Why do we study this model?

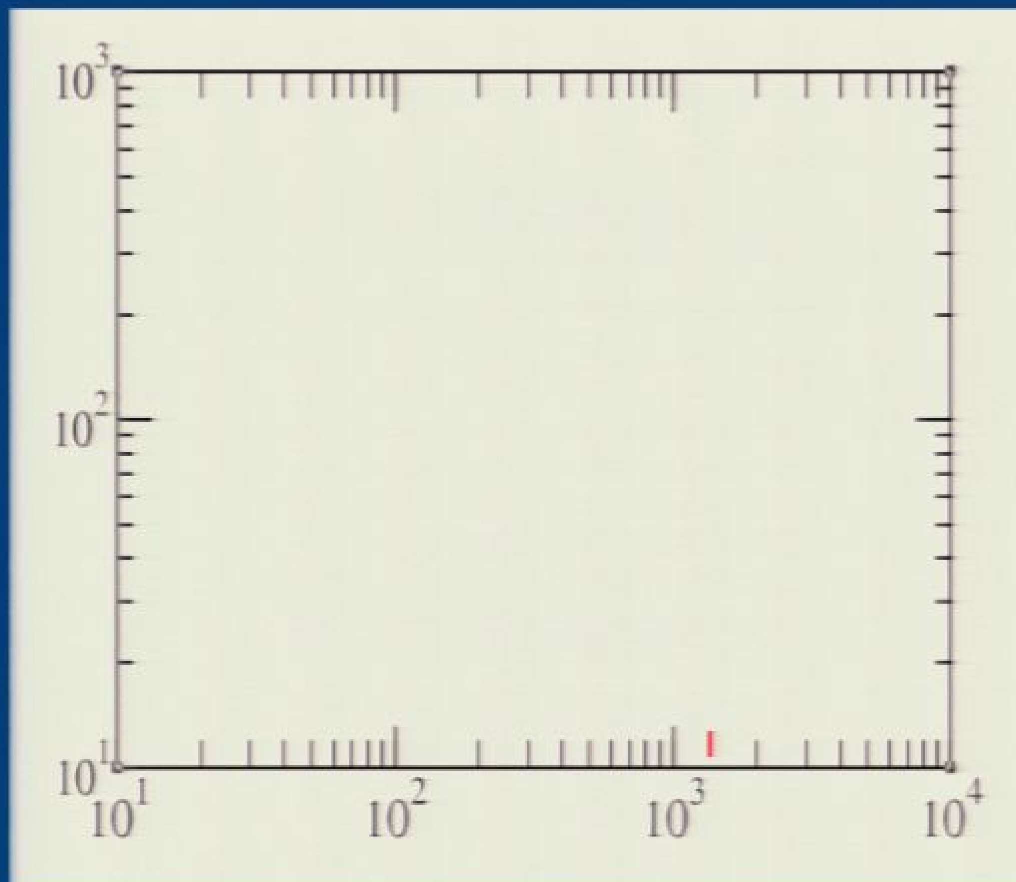
Structures founded in the simulation



- Free state

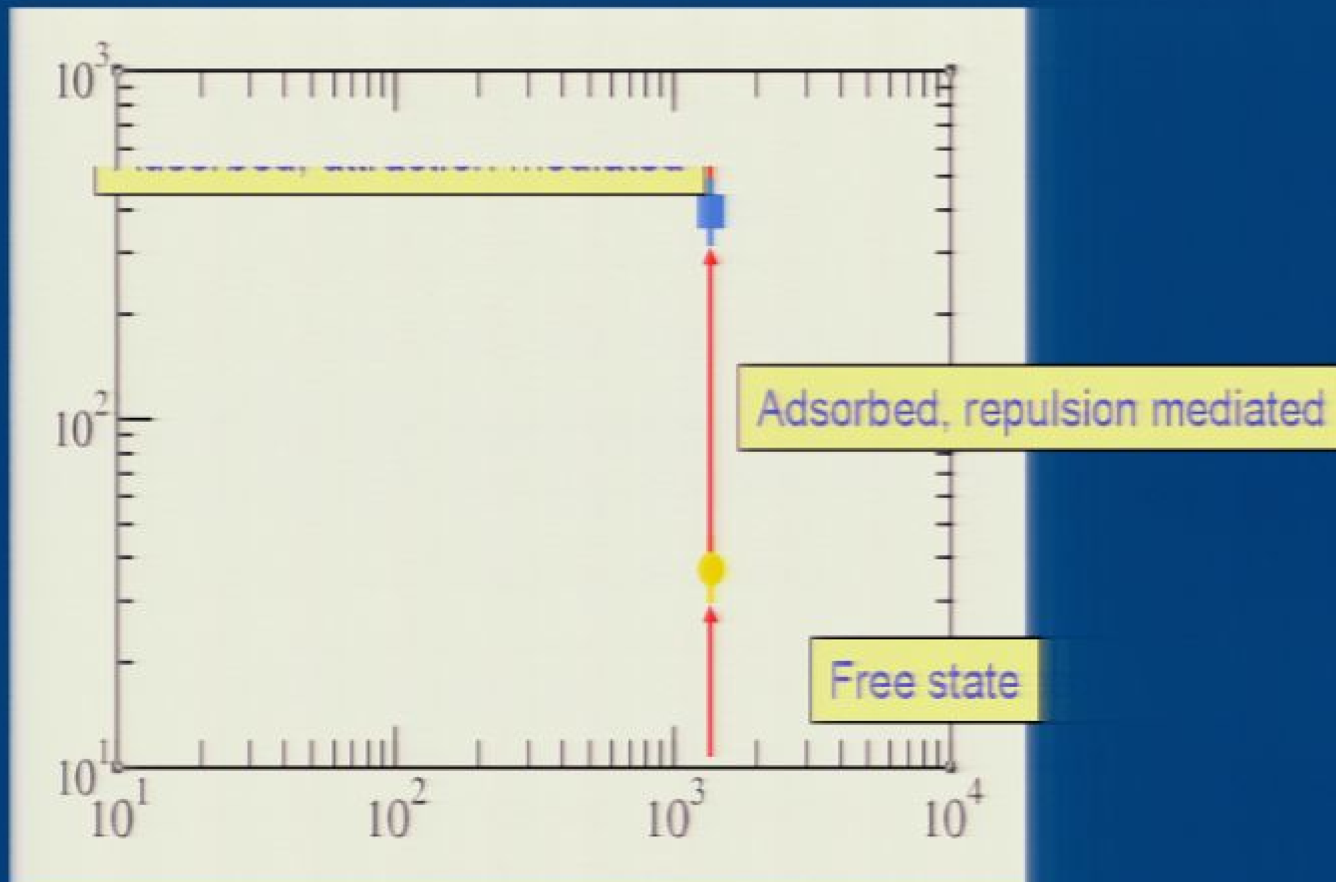
State diagram

$\beta w R^2$



$\beta \sigma R^2$

State diagram

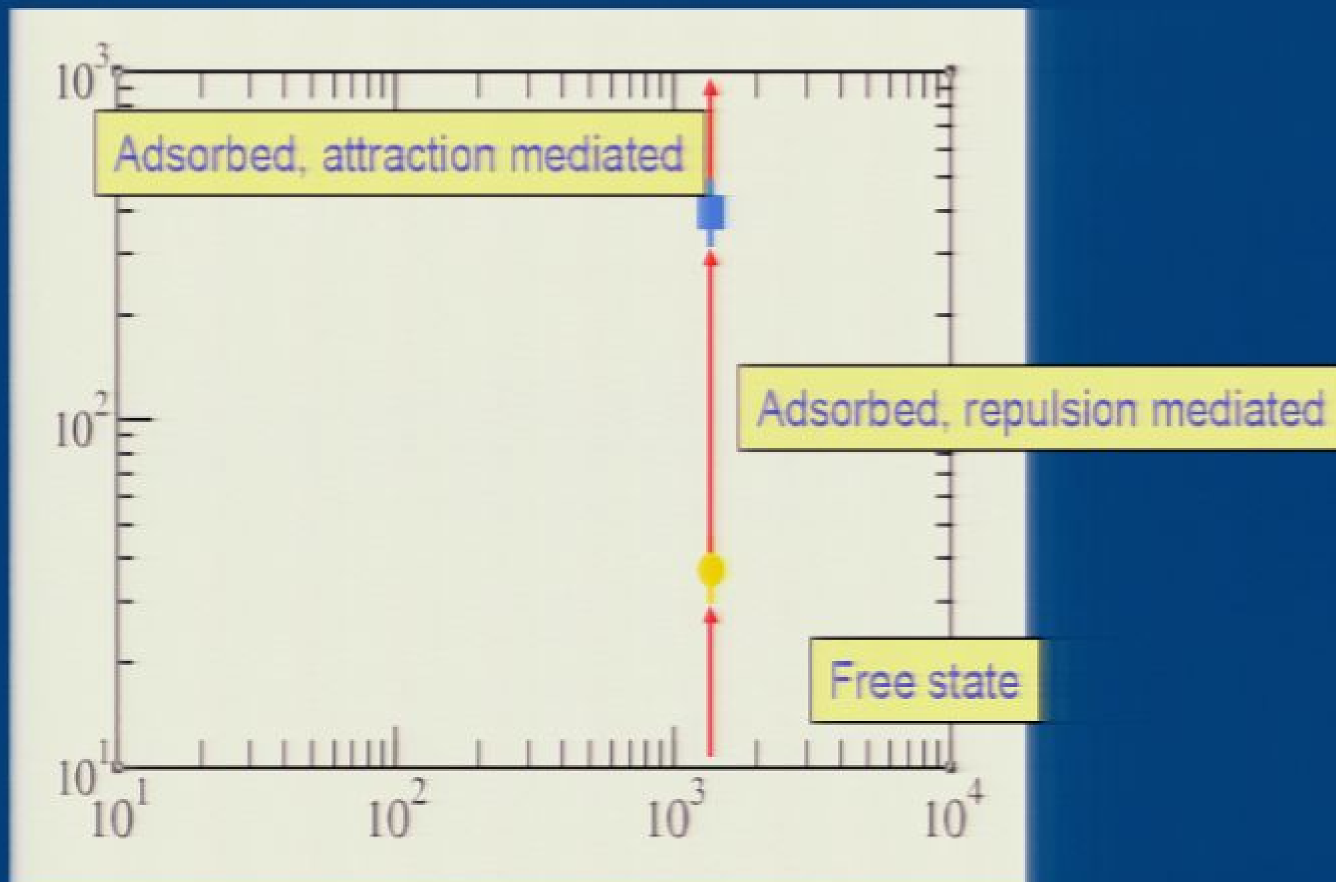


$\beta w R^2$

$\beta \sigma R^2$

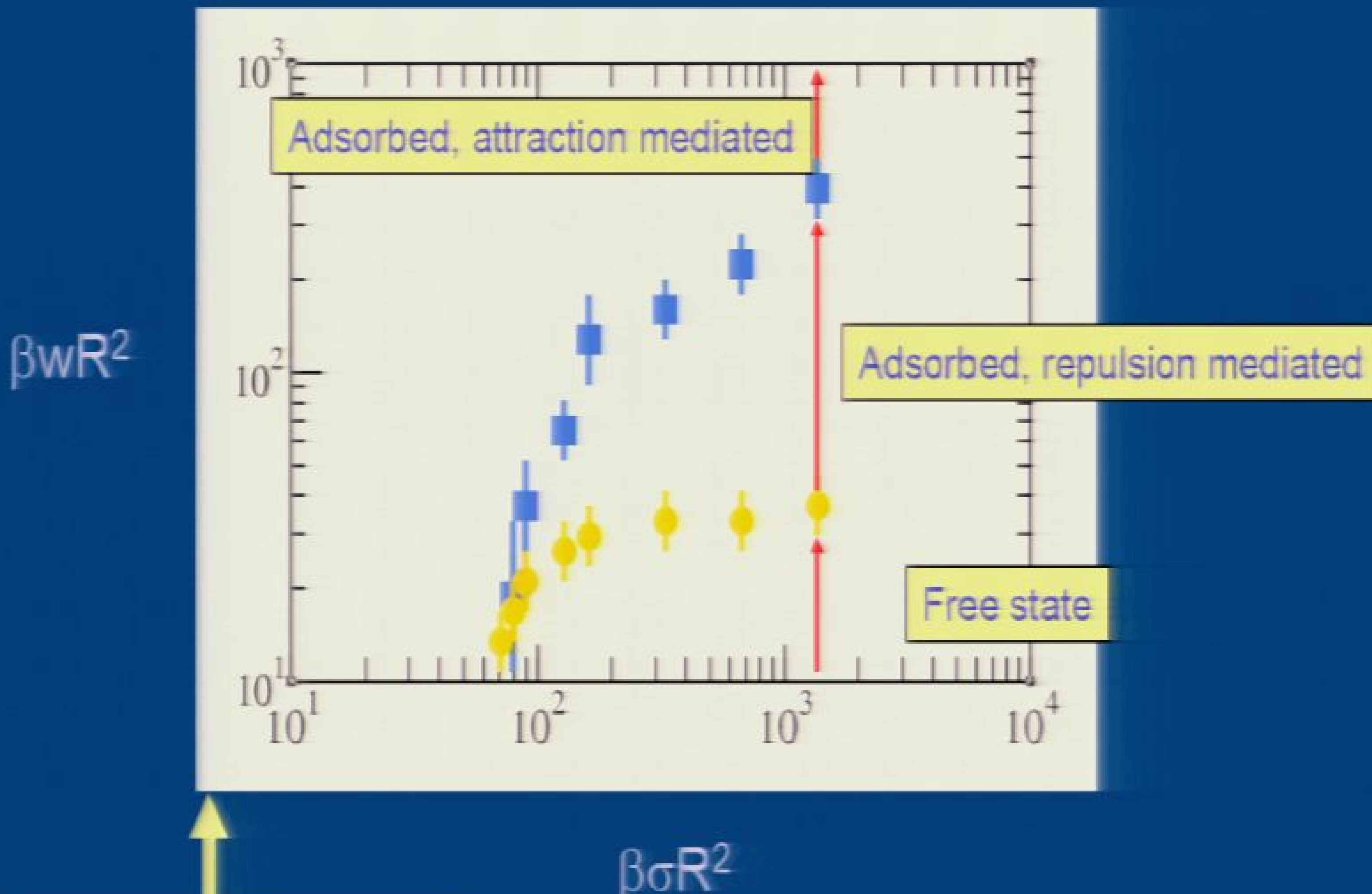
State diagram

$\beta w R^2$



$\beta \sigma R^2$

State diagram



A total of 40 CPU years...

Transition from free to adsorption states

Helfrich energy = $\Delta A\,[\sigma + (\kappa/2)\,(1/r_1+1/r_2)^2\,]$

$\beta F = -\beta w A$

- Adsorption energy

$+\ \beta\sigma R^2\,(A^2/4\pi R^4)$

- Free energy change due to surface stretching

$+\ (\beta\kappa/2)\,(2/R)^2 A$

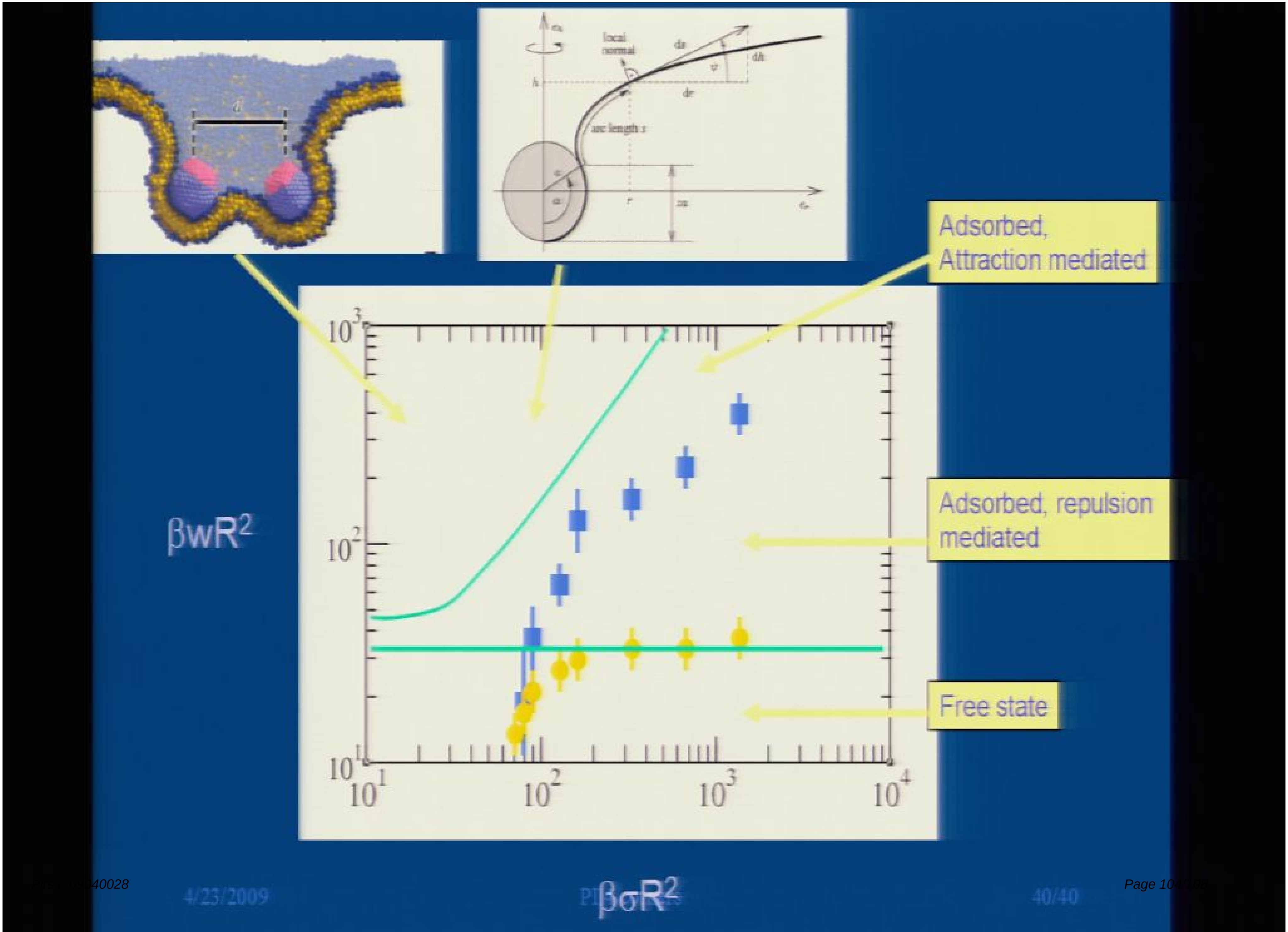
- surface bend

$+\ \ldots$

- F of unadsorbed part; fluctuations

→ $\beta w R^2 = 2\beta\kappa$ free-to-adsorption transition

SUMMARY

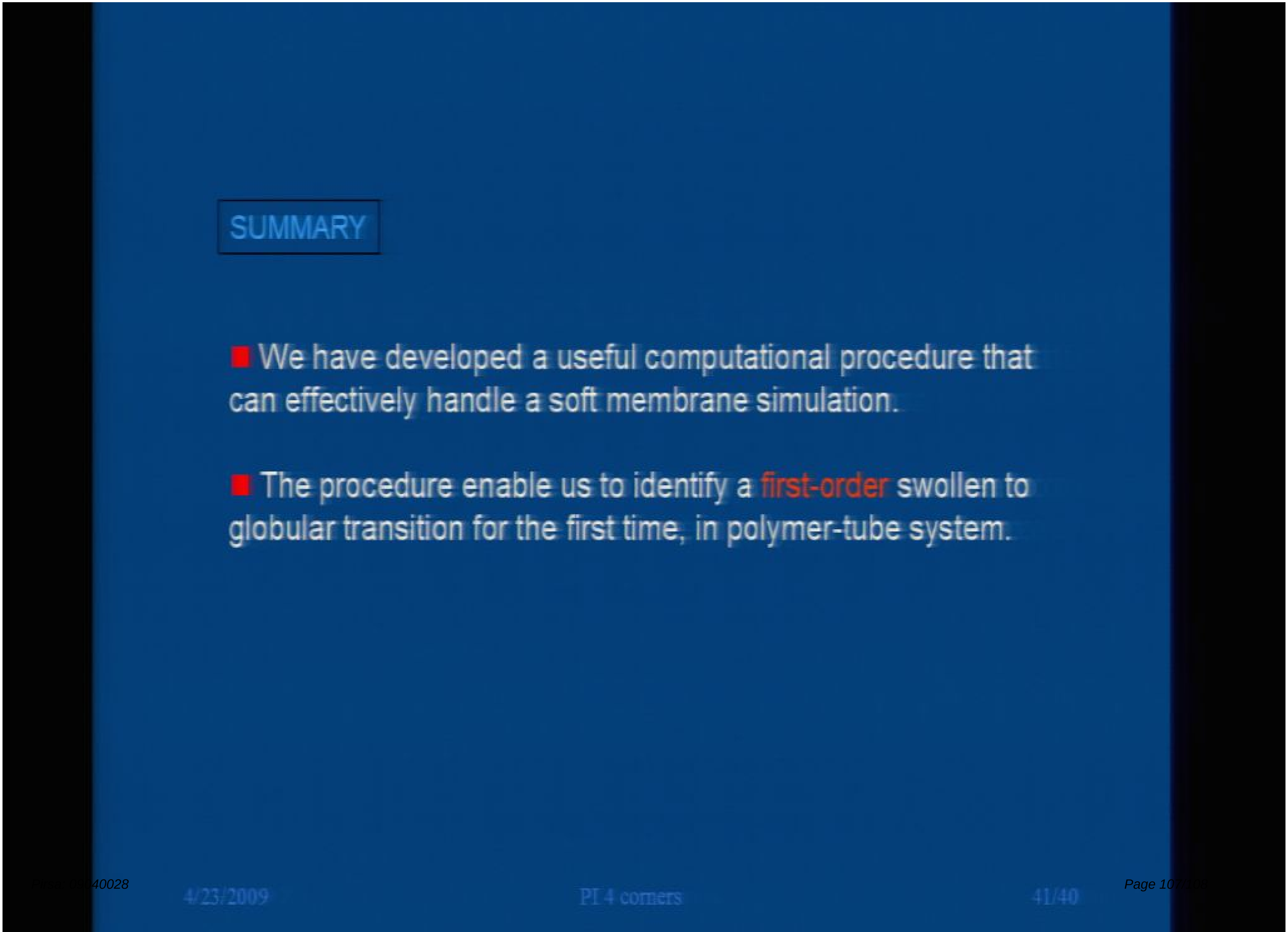


Adsorbed,
Attraction mediated
Adsorbed, repulsion
mediated
Free state
$\beta w R^2$
$\beta \sigma R^2$
10^1
10^2
10^3
10^4
local normal
arc length s
4/23/2009
40/40

SUMMARY

SUMMARY

- We have developed a useful computational procedure that can effectively handle a soft membrane simulation.


SUMMARY
We have developed a useful computational procedure that can effectively handle a soft membrane simulation.
The procedure enable us to identify a first-order swollen to globular transition for the first time, in polymer-tube system.
4/23/2009
PI 4 corners
41/40

SUMMARY

- We have developed a useful computational procedure that can effectively handle a soft membrane simulation.
- The procedure enable us to identify a first-order swollen to globular transition for the first time, in polymer-tube system.
- Understanding a simple membrane/macromolecule system can be theoretically and computationally challenging.