Biopolymers

An introduction into the molecular structure and basic features.

Introduction

- No polymers – no life
- Polymers are the most favorite materials
- Biopolymers are produced in huge amounts

Some numbers

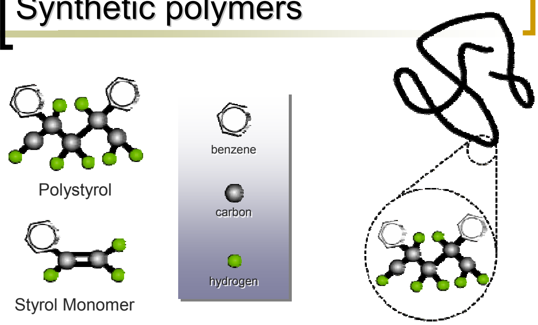
Material	Hauptsächliche Polymer-komponenten	Jahresverbrauch in Tonnen (Welt)	Kilogramm/ Kopf (Welt)	Kilogramm/ Kopf (USA)
Brennholz	Celluose, Lignin	600.000.000	113	250
Papier	Celluose	400.000.000	75	560
Baumwolle	Celluose	14.300.000	2,7	5,6
Kunststoffe	versch. synthetische	54.500.000	12,0	113

H.-G. Elias, Polymere, Seite 3, (1996)

Nobel.se

- Staudinger, Nobelpreis 1953
- Debye, Kuhn und Flory, Nobelpreis 1974
- de Gennes, Nobelpreis 1991

Synthetic polymers



Monomer building blocks

Chainlike macromolecules

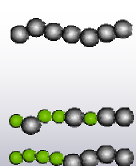
Types of polymers

homopolymer

heteropolymer

statistical

block copolymer



dispersity

monodisperse → some biopolymers

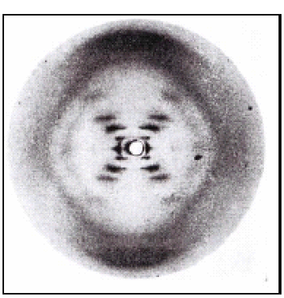
polydisperse → most polymers

Examples for polymers

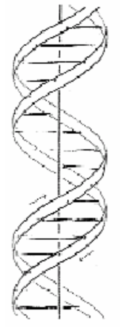
- PVC (Polyvinylchlorid)
- PA (Polyamid)
- PS (Polystyrol)
- Proteins
- Filaments of the cytoskeleton
- DNA, RNA
- Kohlenhydrate (Celluose, Holz, Papier)

DNA structure & elastictiy

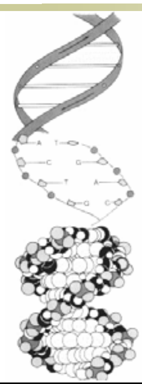
R. Franklin (1920-1958)



Watson & Crick



DNA – a multi-functional molecule



Elastizität

(Biegen & Verdrillen)

Genetische Information

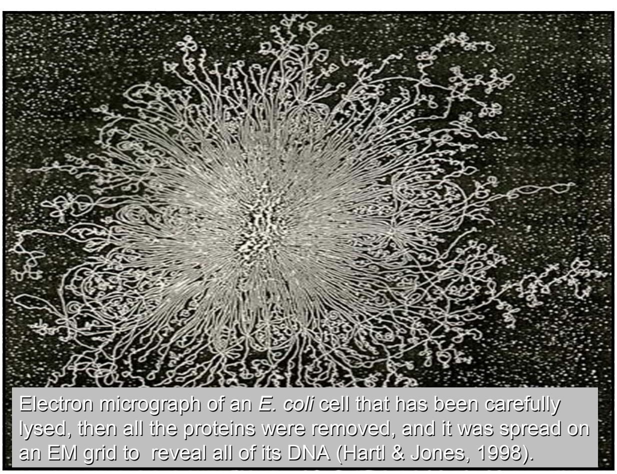
(ACTG)

Spezifische Wechselwirkungen

(Substrat & Molekulare Schiene)

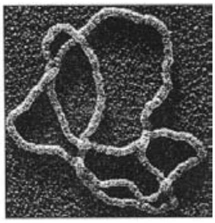
Unspezifische Wechselwirkungen

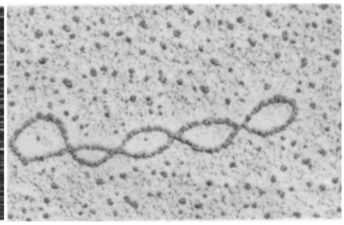
(entropisch & elektrostatisch)



Electron micrograph of an *E. coli* cell that has been carefully lysed, then all the proteins were removed, and it was spread on an EM grid to reveal all of its DNA (Hartl & Jones, 1998).

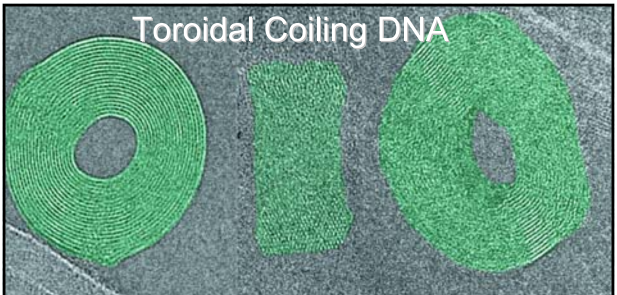
DNA knots and supercoils

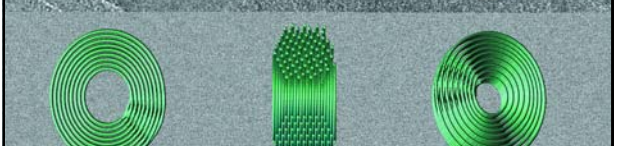




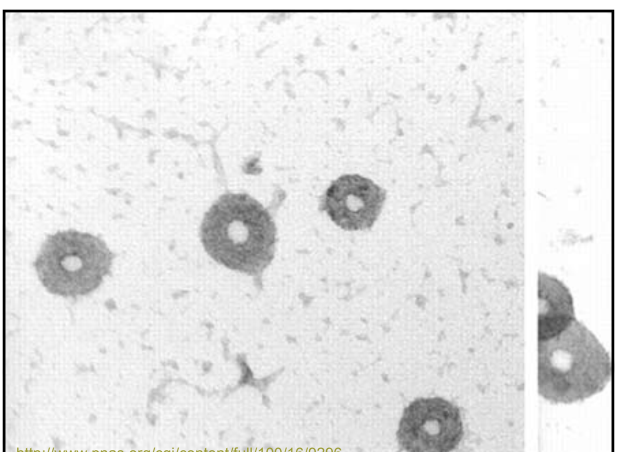
DNA-knot: Wassermann and Cozzarelli, Science 229 (1985)

Toroidal Coiling DNA

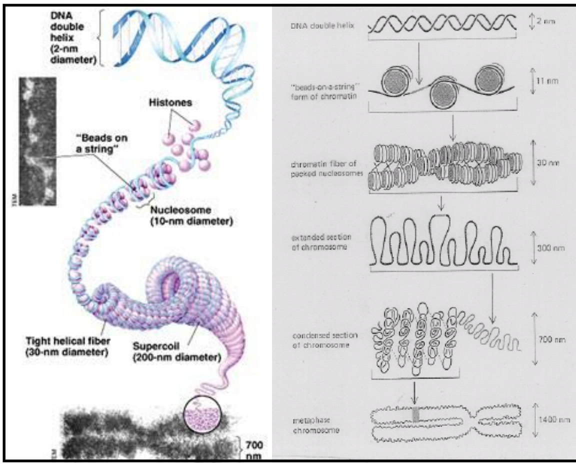




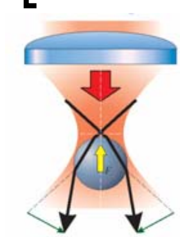
http://www-vis.lbl.gov/Vignettes/KDowning-DNA/



http://www.pnas.org/cgi/content/full/100/16/9296

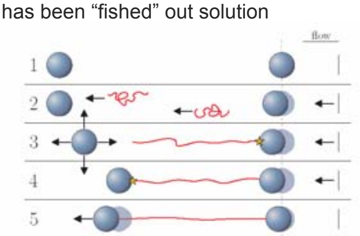


Optical tweezers

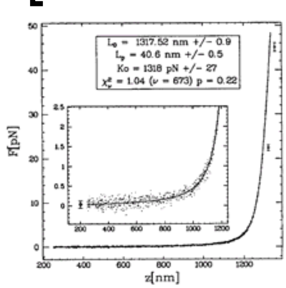


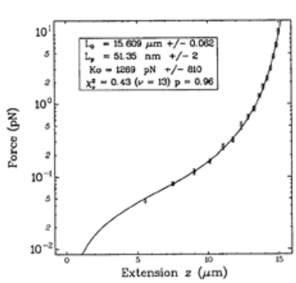
Optical Tweezers are commonly used for stretching DNA

Experiments start after a DNA molecule has been "fished" out solution



Stretching DNA Molecules



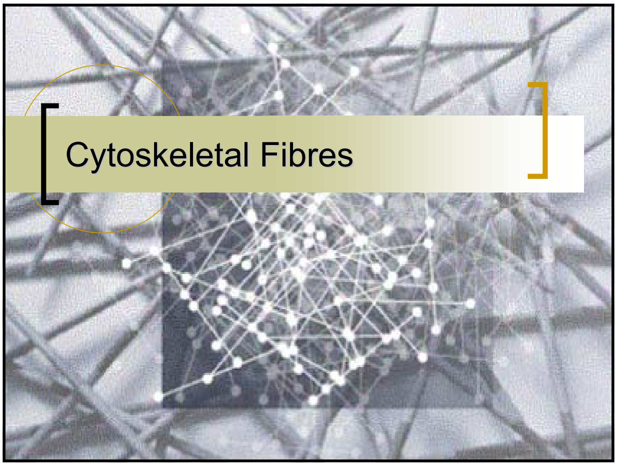


M.D. Wang et al., Biophys. J. 72, 1335 (1997)

T.R. Strick et al., Science 271, 1835 (1996)

Question

- How should one describe the conformations and dynamics of DNA?
- Response to external forces?
- Interactions?
- (Self-)organization?
- Sequence specificity?
- ...



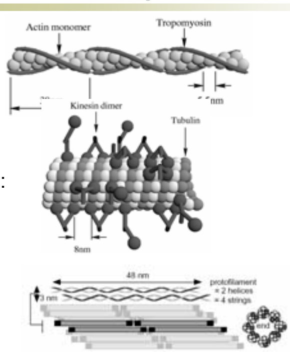
Cytoskeletal Fibres

Fibres of the Cytoskeleton

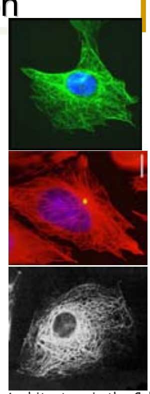
F-Aktin:

Microtubules:

Intermediate Filaments:

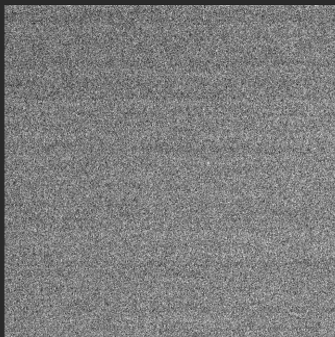


Cartoon



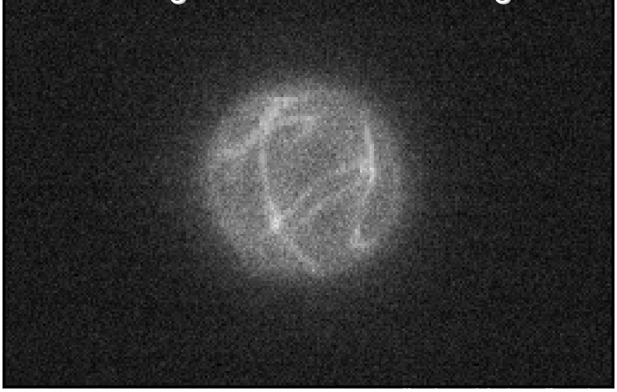
Architecture in the Cell

Fluctuation Analysis of Microtubules

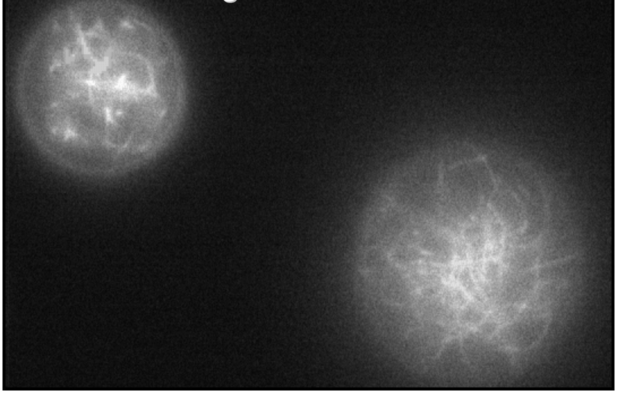


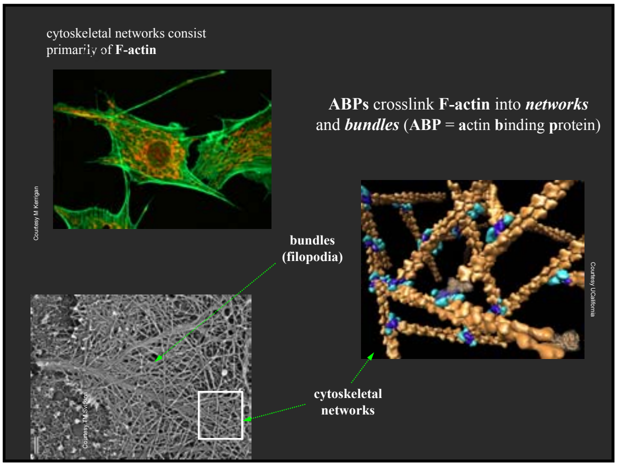
F. Pampaloni et al., q-bio/0503037

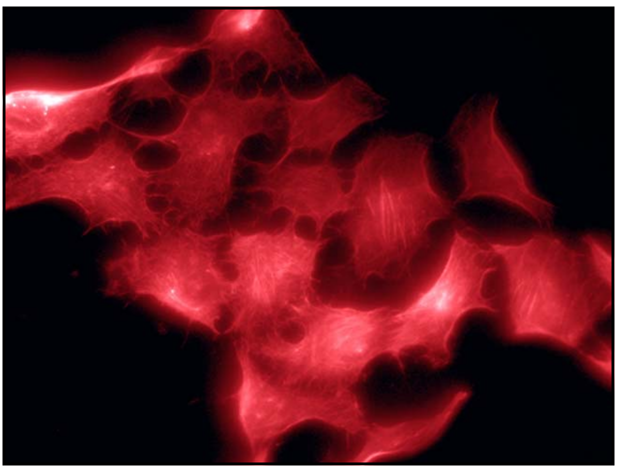
Strong confinement of strings



.. or strings in a mini-universe?







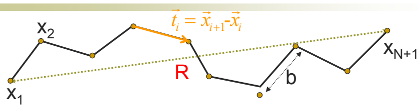
My favorite movie ☺

See Tom Stossel's web page: http://expmed.bwh.harvard.edu/

Single Filaments

Gaussian Chains
Semiflexible Chains

The Freely Jointed Chain Model



$$\langle \vec{R} \rangle = \langle \vec{x}_{N+1} - \vec{x}_1 \rangle = \left\langle \sum_{i=1}^{N} \vec{t}_i \right\rangle = \sum_{i=1}^{N} \langle \vec{t}_i \rangle = 0$$

$$\langle \vec{R}^2 \rangle = \langle (\vec{x}_{N+1} - \vec{x}_1)^2 \rangle = \left\langle \left(\sum_{i=1}^{N} \vec{t}_i \right)^2 \right\rangle = \sum_{i=1}^{N} \langle \vec{t}_i^{\,2} \rangle = N b^2$$

The root mean-square end-to-end distance grows like the square root of the degree of polymerization N

$$\sqrt{\langle R^2 \rangle} = b\sqrt{N}$$

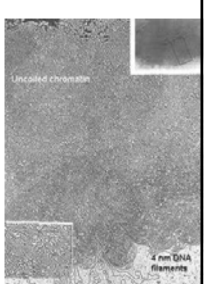
How large is a DNA Molecule?

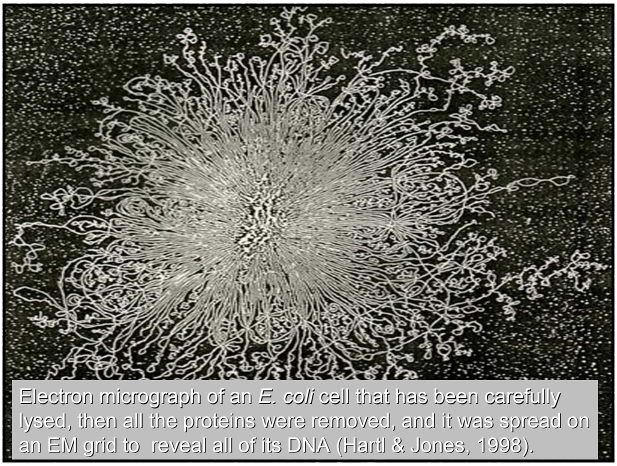
Contour length can be up to L = 1m

Length of a "monomer": b = 100 nm = 10^{-7} m

Typical Size: R ~ 0.03 cm

Note that this is still far too big to squeeze into a cell nucleus, which is about 10^{-6} m in diameter!





Electron micrograph of an *E. coli* cell that has been carefully lysed, then all the proteins were removed, and it was spread on an EM grid to reveal all of its DNA (Hartl & Jones, 1998).

Animations of Polymer Statistics

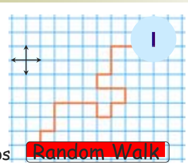
GIANT MOLECULES MOVIES

A.Y. Grosberg and A.R. Khokhlov, *Giant Molecules*, Academic Press (San Diego, 1997).

With CD-ROM by S.V. Buldyrev and V.S. Pande

End-to-End Distribution Function

bond vectors $\vec{b}_i$



Cubic lattice:

coordination number z=6

P(R,N) = probability to find a end-to-end distance R after N steps

Configuration of a freely jointed chain

$$P(\vec{R},N)=\frac{1}{z}\sum_{i=1}^{z}P(\vec{R}-\vec{b}_i,N-1)$$

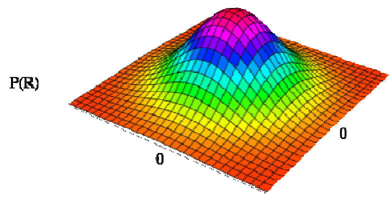
For $N>>1$: $P(\vec{R}-\vec{b}_i,N-1)=P(\vec{R},N)-\frac{\partial P}{\partial N}-\frac{\partial P}{\partial R_i^\alpha}b_i^\alpha+\frac{1}{2}\frac{\partial^2 P}{\partial R_i^\alpha \partial R_j^\beta}b_i^\alpha b_j^\beta$

$$\frac{\partial P}{\partial N}=\frac{b^2}{6}\frac{\partial^2 P}{\partial \vec{R}^2}$$ diffusion equation

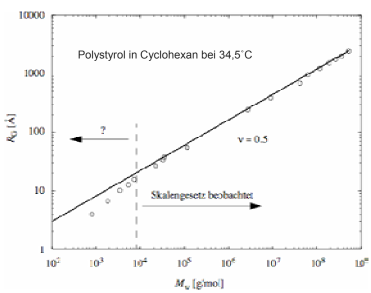
End-to-End Distribution Function

… a Gaussian with width ~ $N^{1/2}$

$$\frac{\partial P}{\partial N} = \frac{b^2}{6}\frac{\partial^2 P}{\partial \vec{R}^2} \Leftrightarrow P(R,N) = \left(\frac{3}{2\pi N b^2}\right)^{3/2} \exp\left[-\frac{3R^2}{2Nb^2}\right]$$

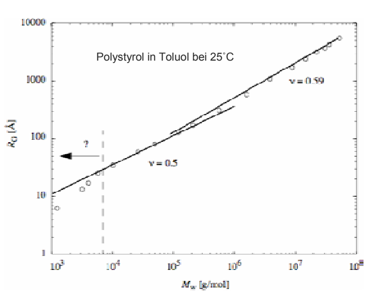


Experiment I



K. Huber et al., Macromolecules 18 (7), 1461 (1985)

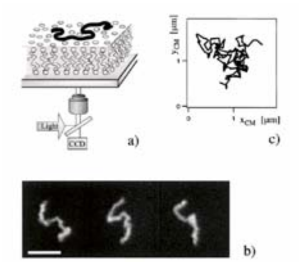
Experiment II

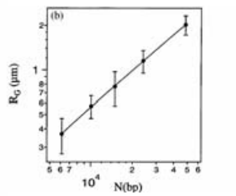


K. Huber et al., Macromolecules 18 (7), 1461 (1985)

Excluded Volume Effects

Single DNA Molecules confined to 2D

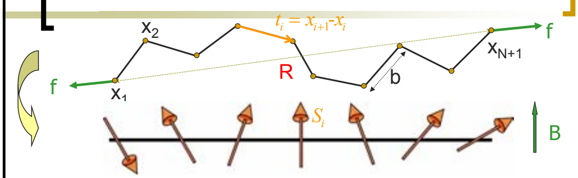




$R_G \sim N^{3/4}$

B. Maier and J.O. Rädler, PRL 82, 1911 (1999)

Force-extension relation



$$H = -\vec{f}\cdot(\vec{x}_{N+1}-\vec{x}_1) = -\vec{f}\cdot\sum_{i=1}^{N}\vec{t}_i \quad\Leftrightarrow\quad H = -\vec{B}\cdot\sum_{i=1}^{N}\vec{S}_i$$

freely jointed chain — paramagnet

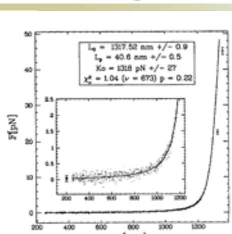
chain extension / magnetization: $R_\parallel := \langle \vec{n}\cdot\vec{R}\rangle = \left\langle \sum_{i=1}^{N}\vec{n}\cdot\vec{t}_i \right\rangle = L\,\mathcal{L}(fb/k_BT)$

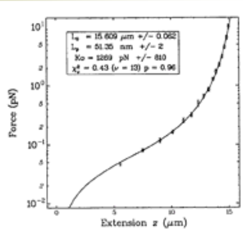
$\mathcal{L}(x) = \coth(x) - 1/x$ Langevin function

Small forces: $R_\parallel = \frac{Nb^2}{3k_BT} f$ Large forces: $R_\parallel = L\left(1-\frac{k_BT}{fb}\right)$

Curie-Weiss law ⇔ Entropy elasticity $k_{eff} \sim T$ Saturation ~ 1/f

Stretching DNA molecules





? ~~$R_\parallel = L\left(1-\frac{k_BT}{fb}\right)$~~ ➡ $R_\parallel = L\left(1-\sqrt{\frac{k_BT}{4fl_p}}\right)$ But why ?

M.D. Wang et al., Biophys. J. 72, 1335 (1997) T.R. Strick et al., Science 271, 1835 (1996)