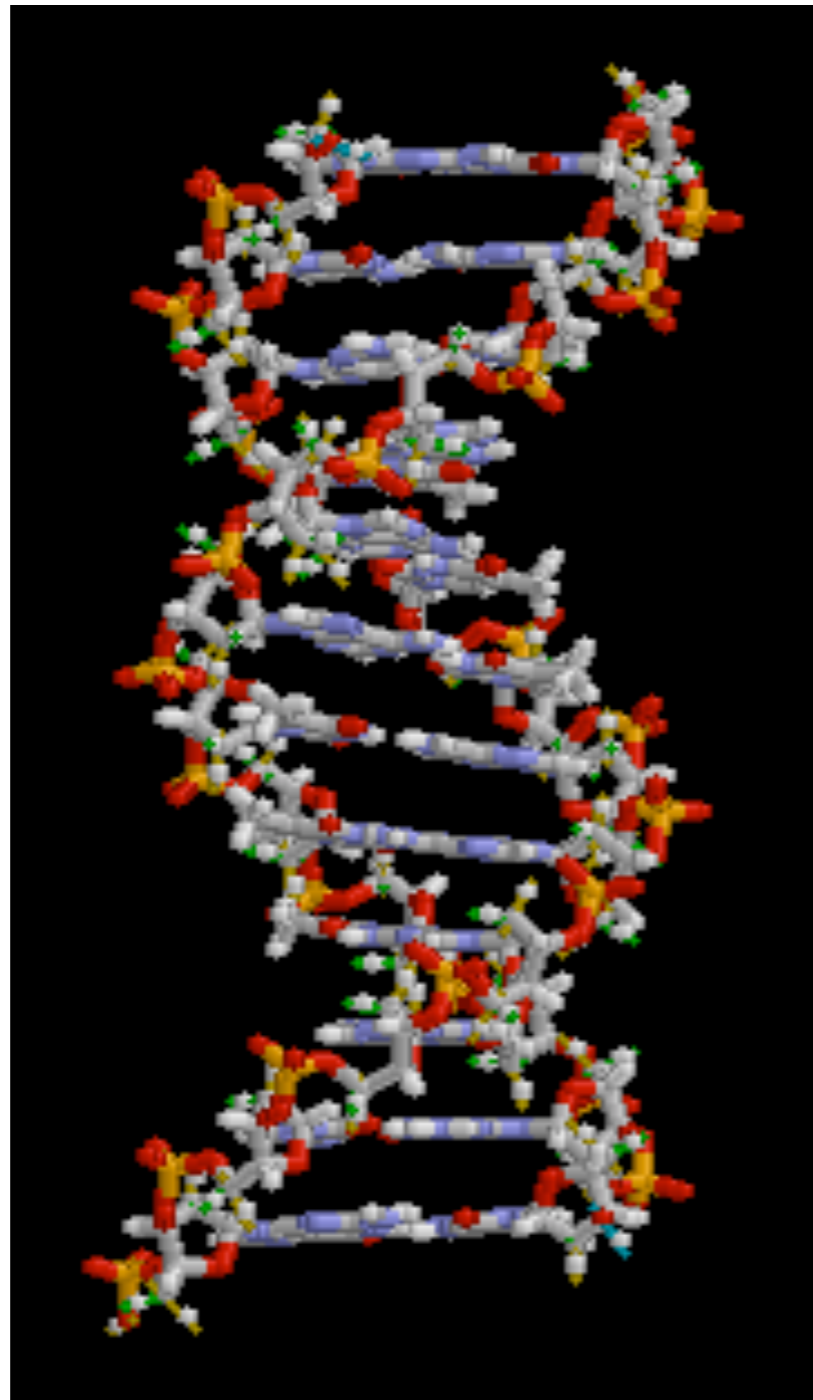


Polymers

18.S995 - L12 & 13

DNA = biopolymer pair

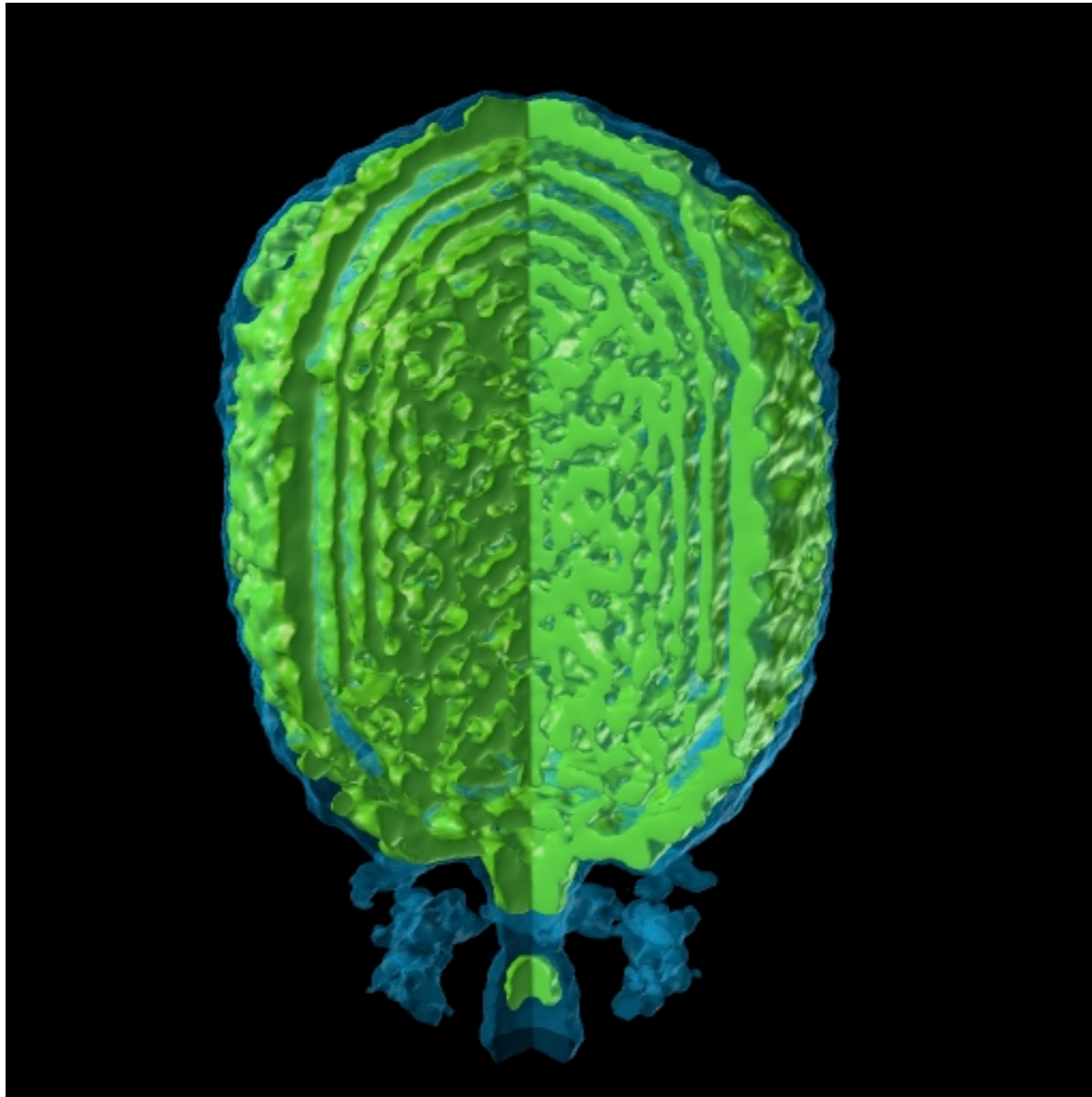


~ 3m per cell

~ 10^{14} cells/human

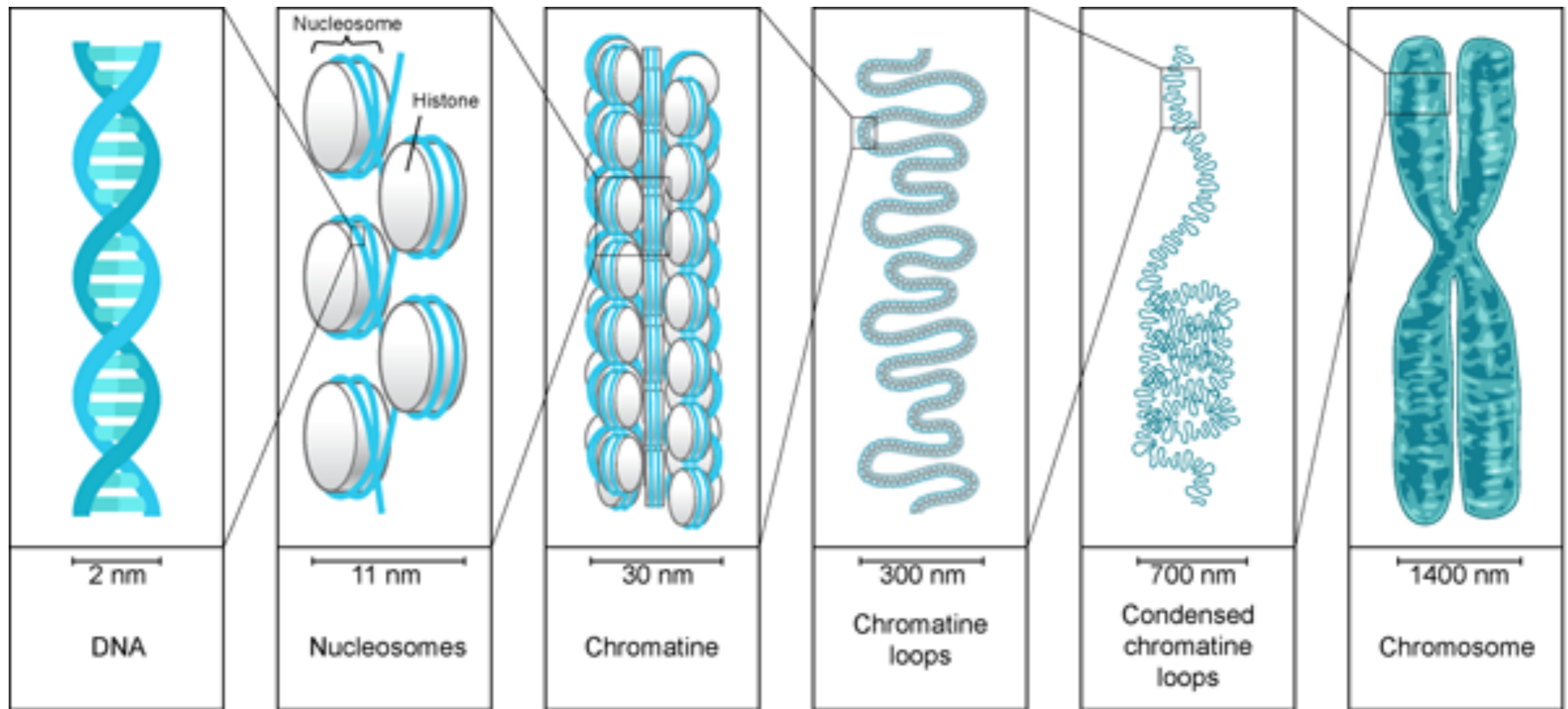
> max. distance between
Earth and Pluto
(~50 AU = 7.5×10^{12} m)

DNA packaging



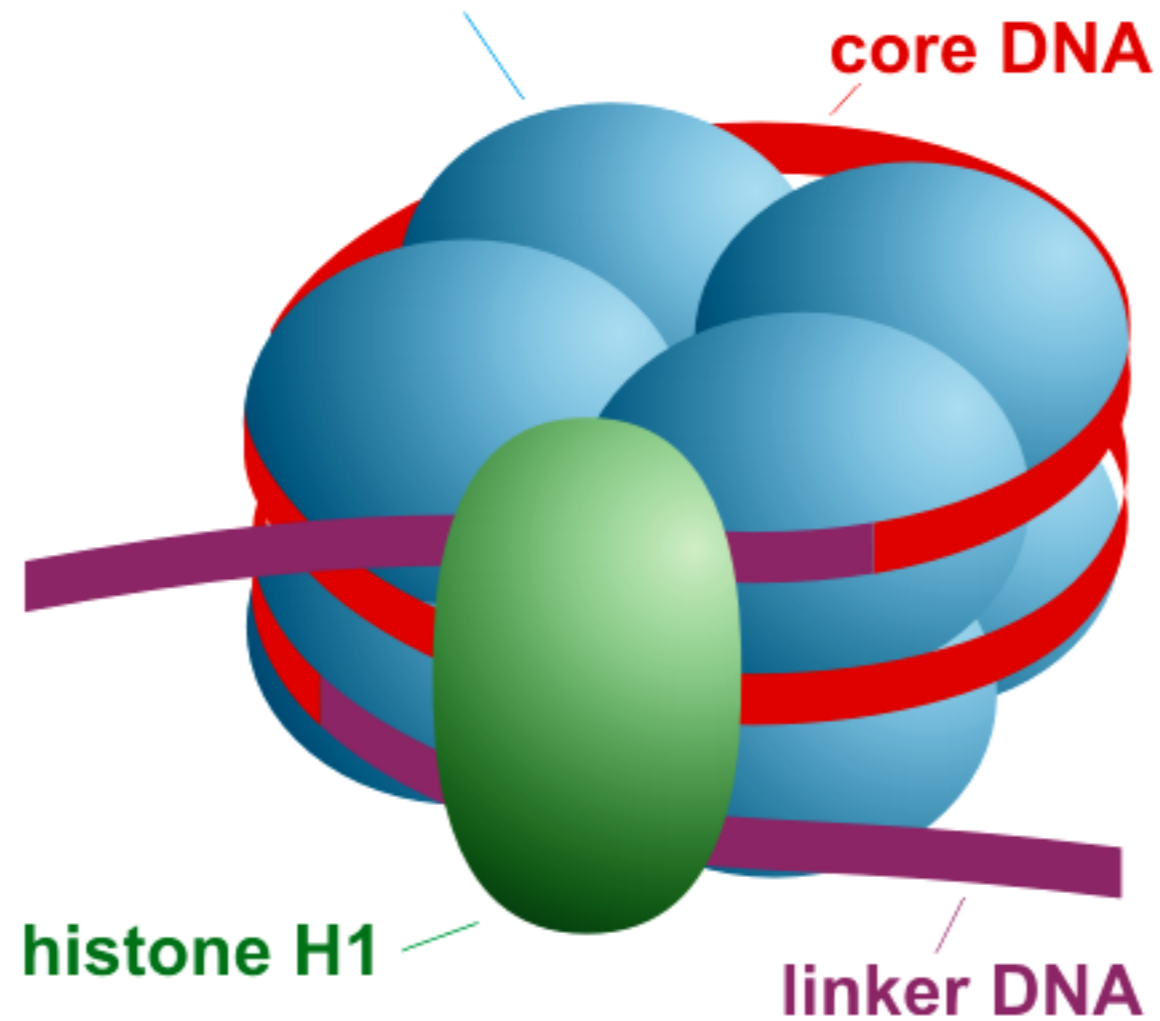
Virus Phi-29

DNA packaging in eukaryotes

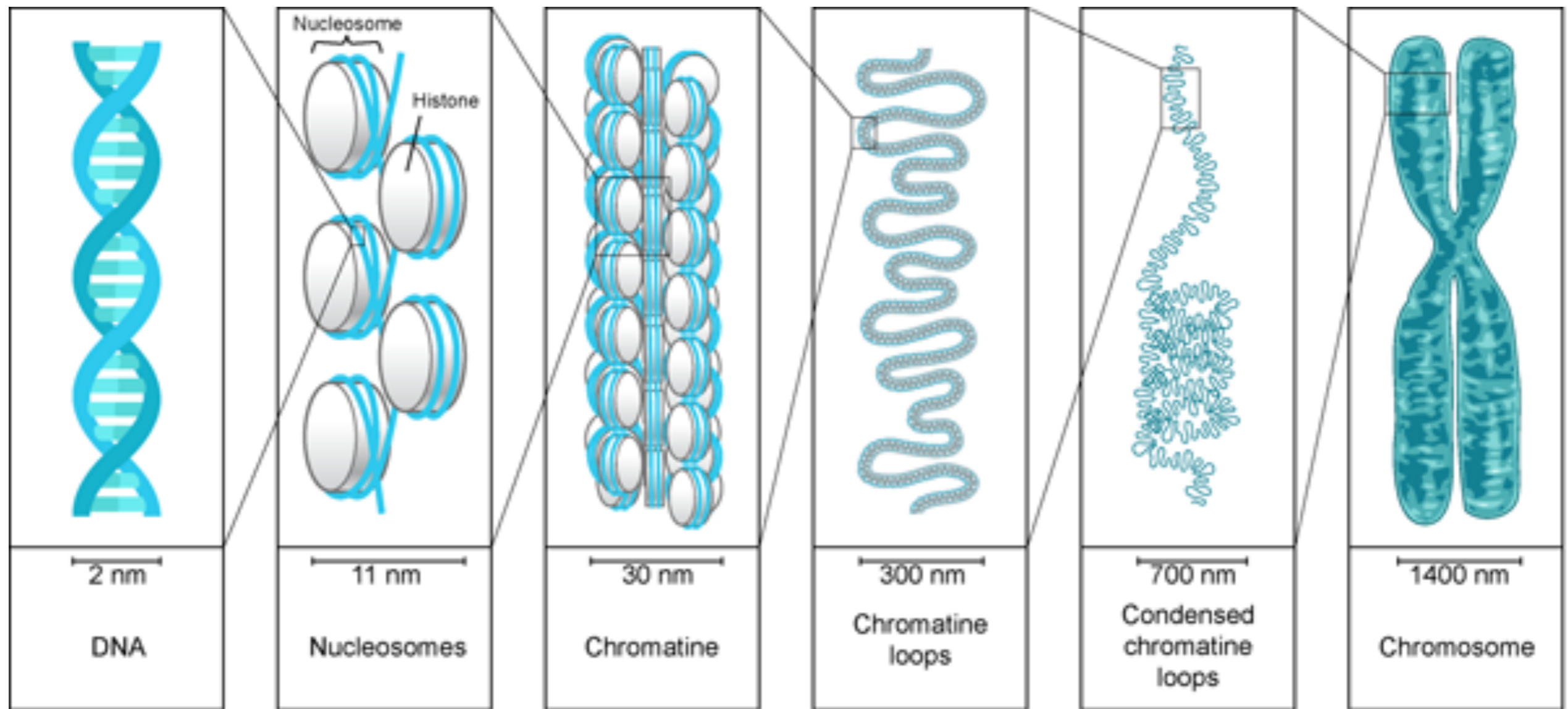


Nucleosomes

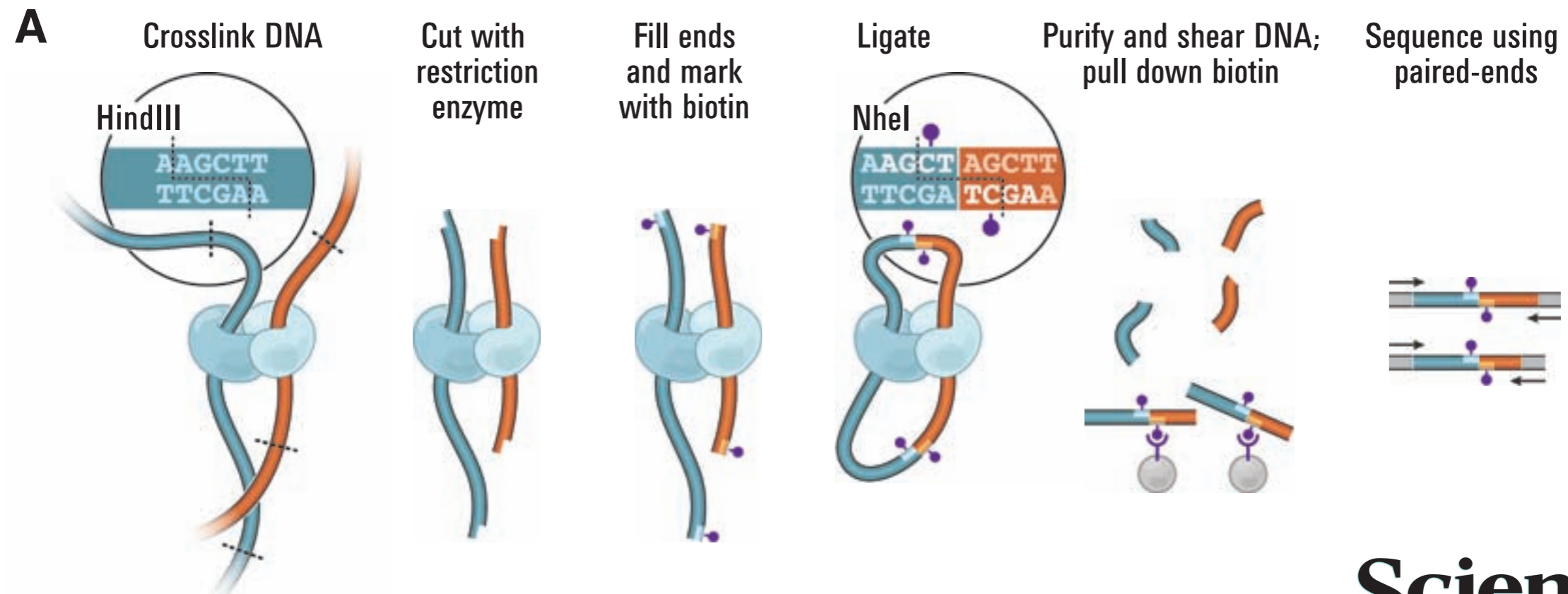
octamer of core histones:
H2A, H2B, H3, H4 (each one $\times 2$)



DNA packaging in eukaryotes



DNA packaging in humans

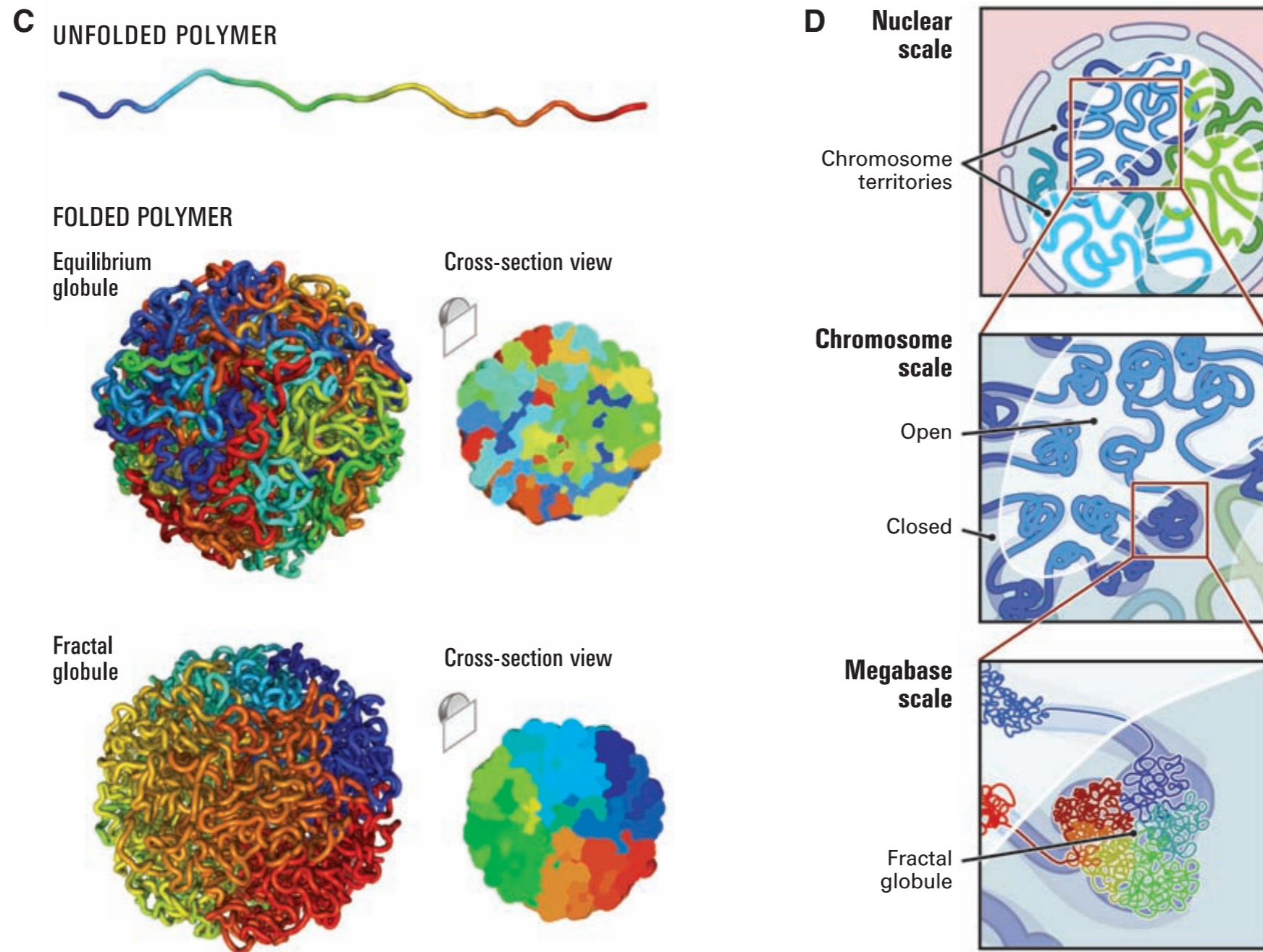


Lieberman-Aiden et al.
(2011) Science



AAAS

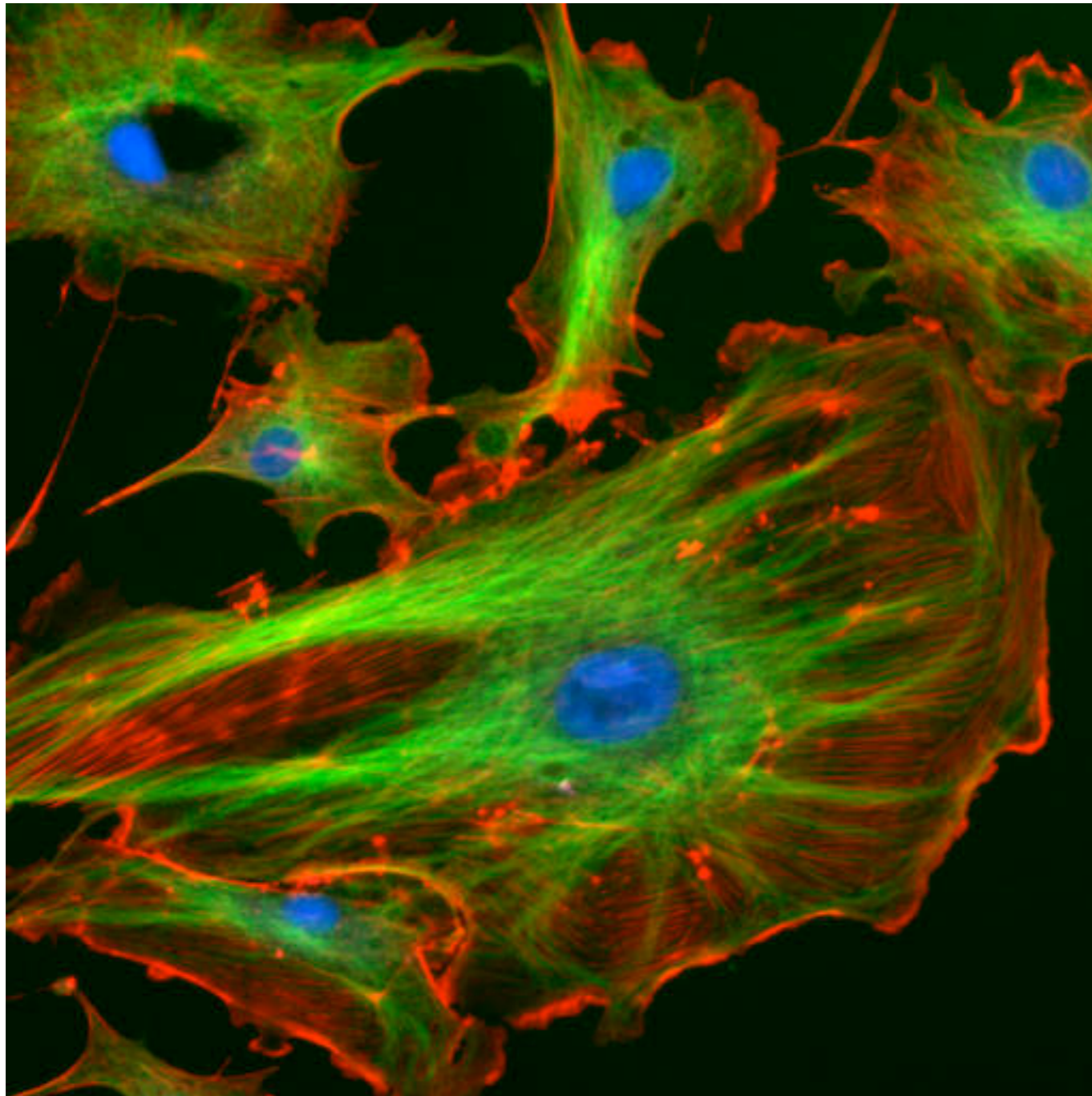
DNA packaging in humans



Lieberman-Aiden et al. (2011) Science

dunkel@math.mit.edu

Cyto-skeleton



Nucleus

Actin

Microtubuli

mechanical properties,
network topology, ...

eukaryotic cells (source: wiki)

Cyto-skeleton

microtubules



25-nm
diameter

actin filaments



7-nm
diameter

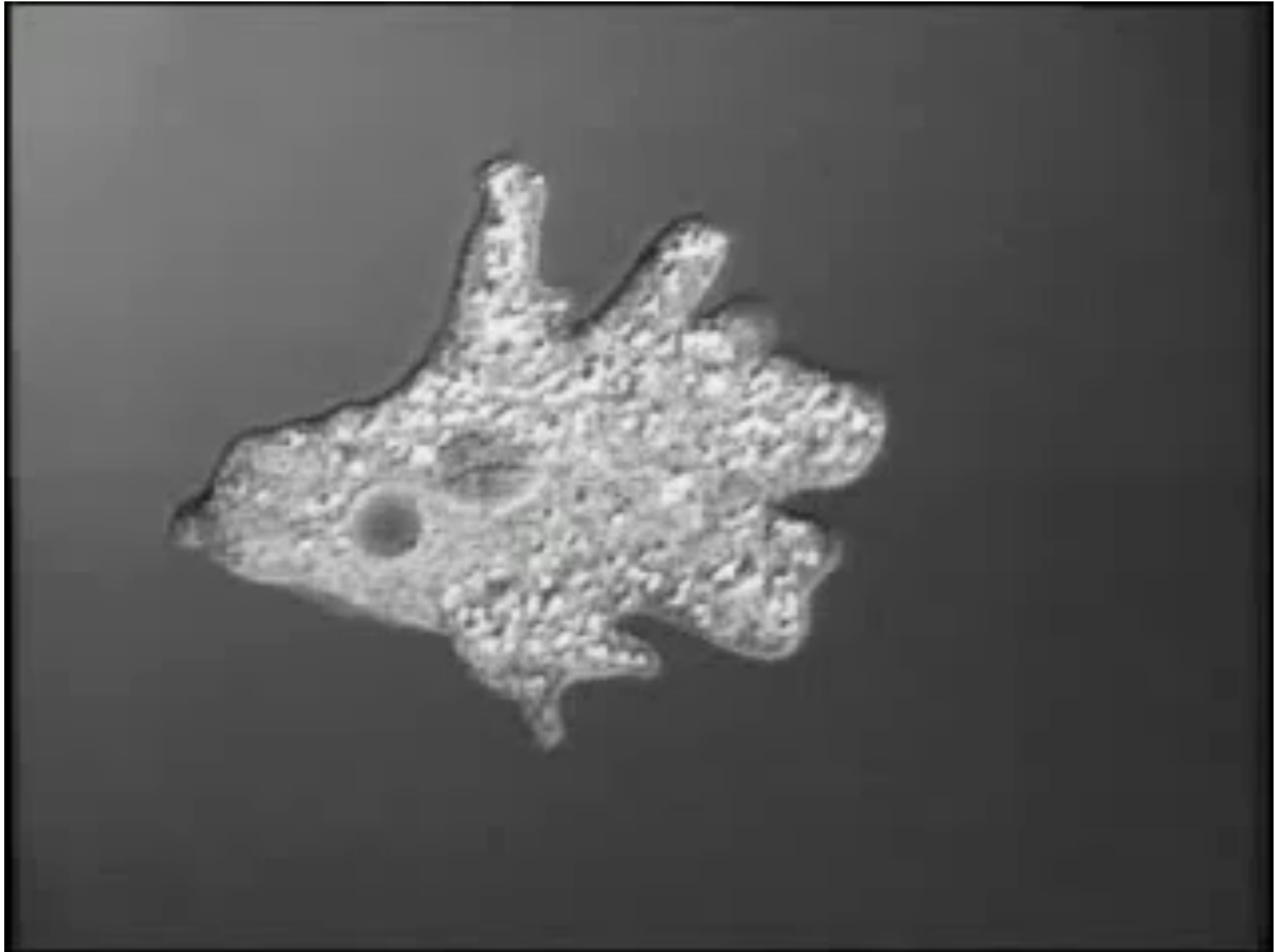
intermediate filaments



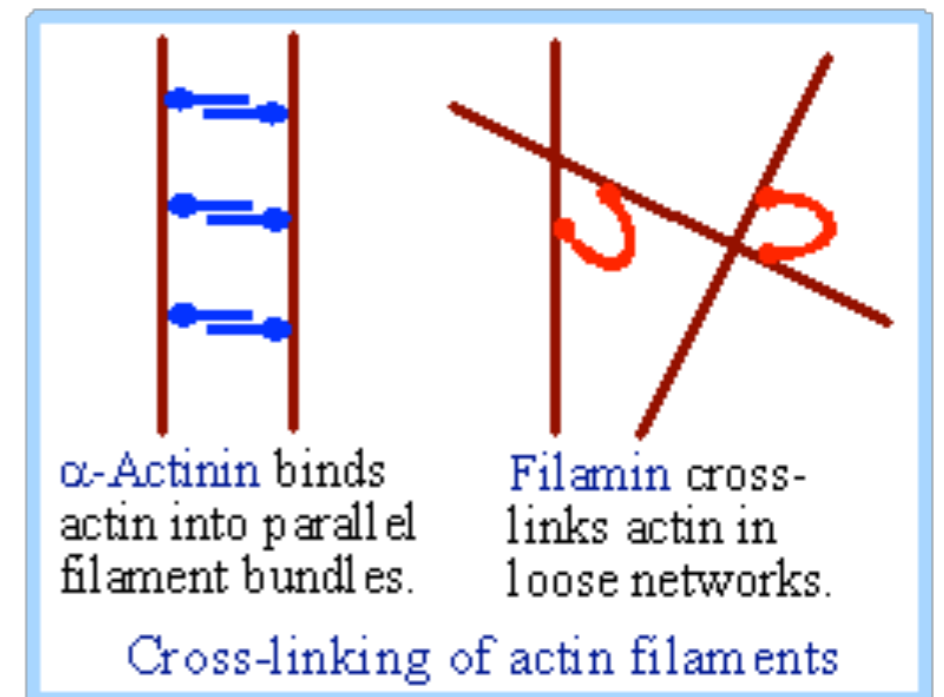
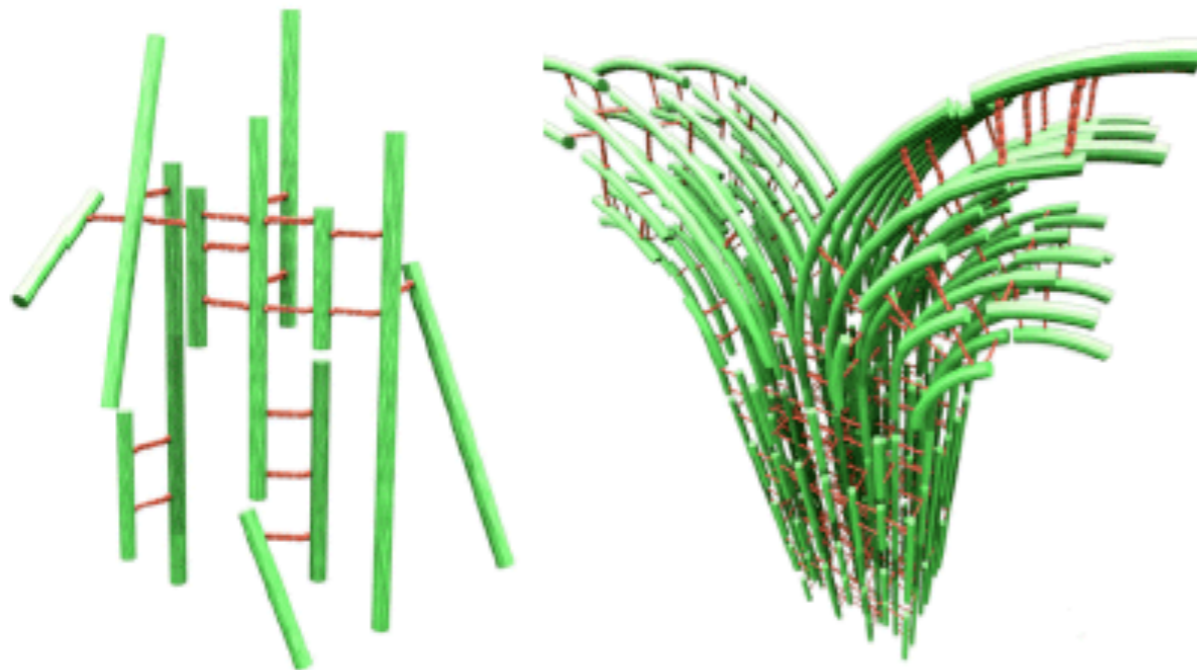
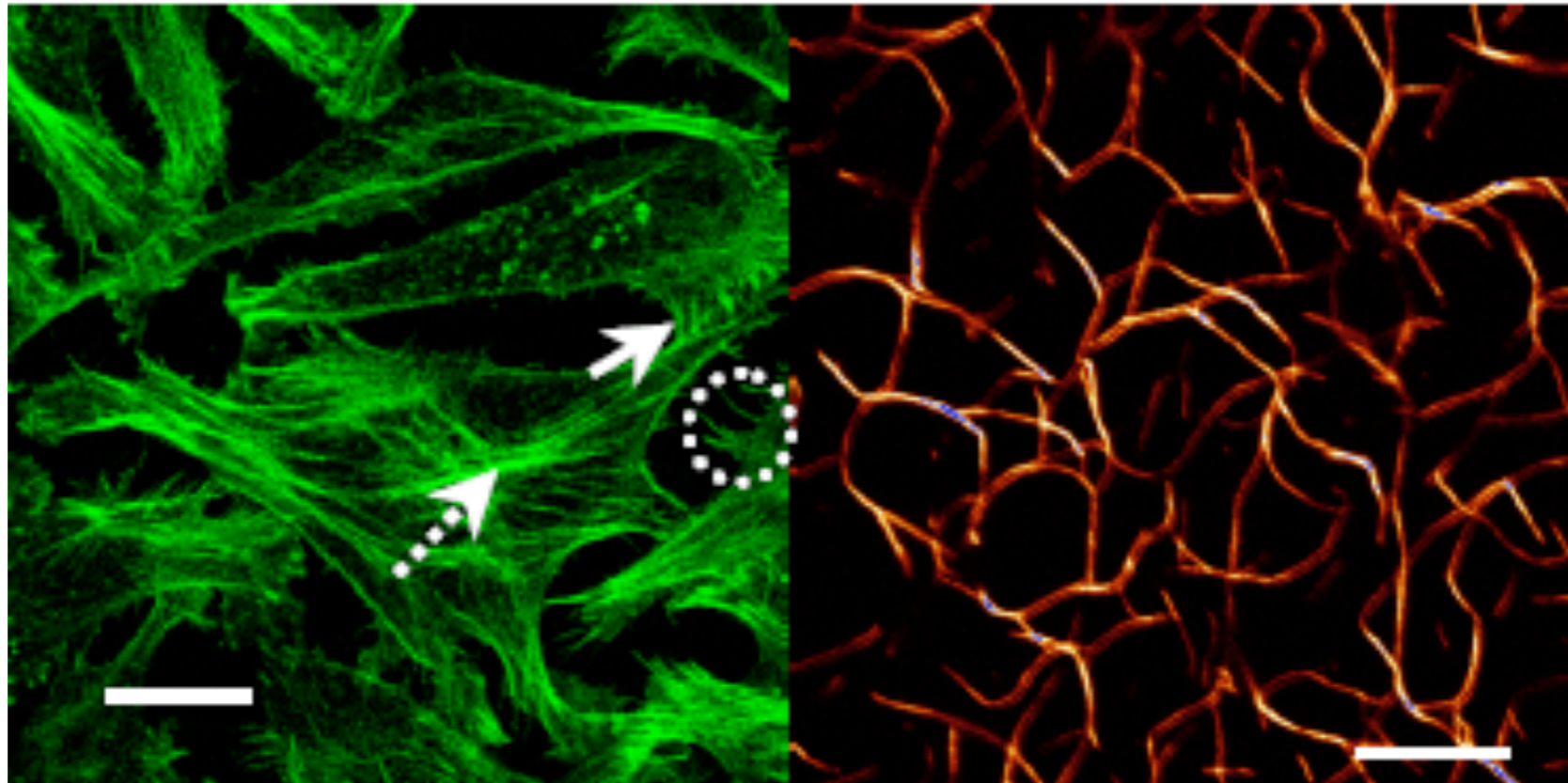
10-nm
diameter

<http://library.thinkquest.org/C004535/cytoskeleton.html>

Amoeba



Actin bundles



Cyto-skeleton

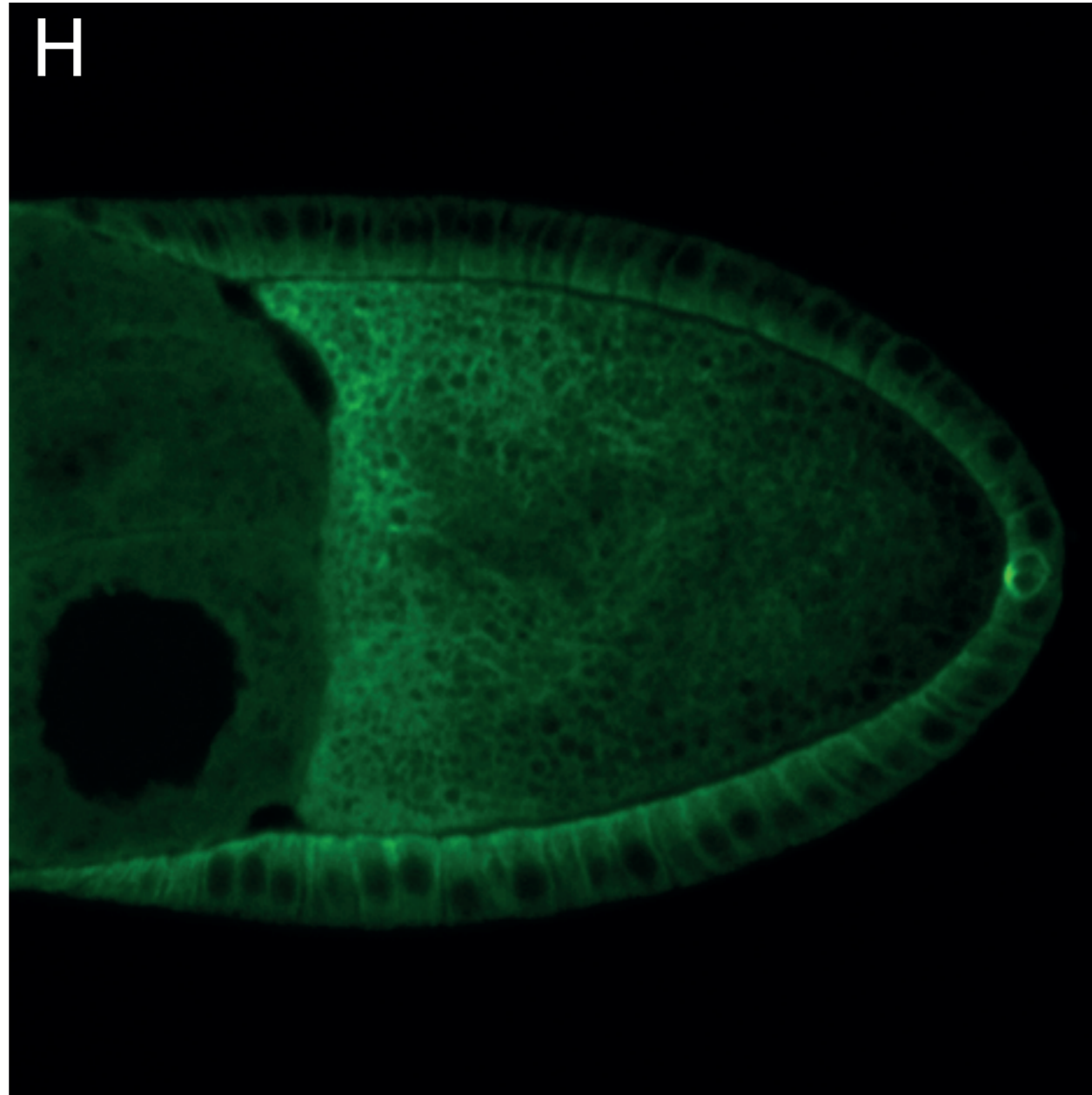
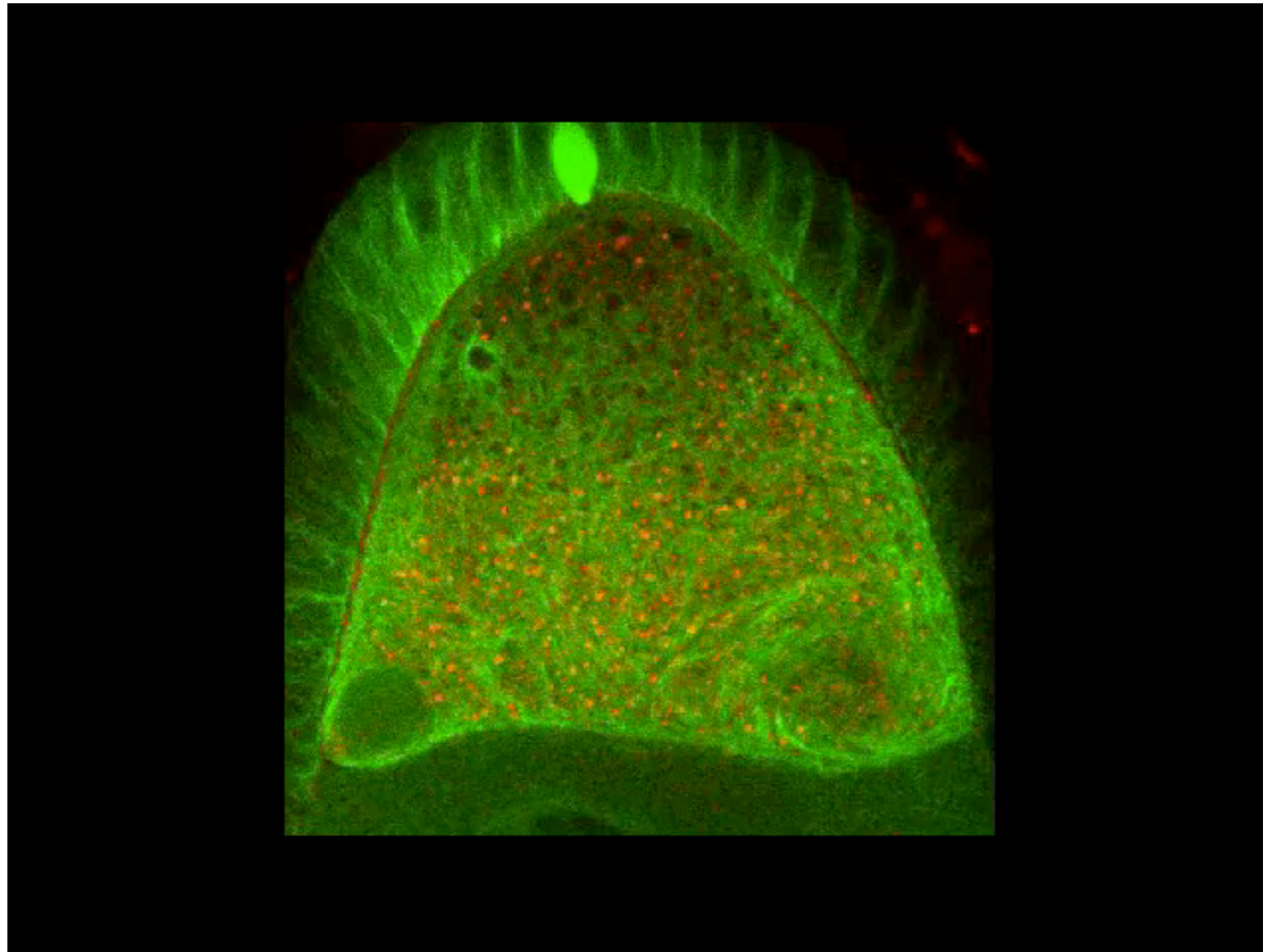


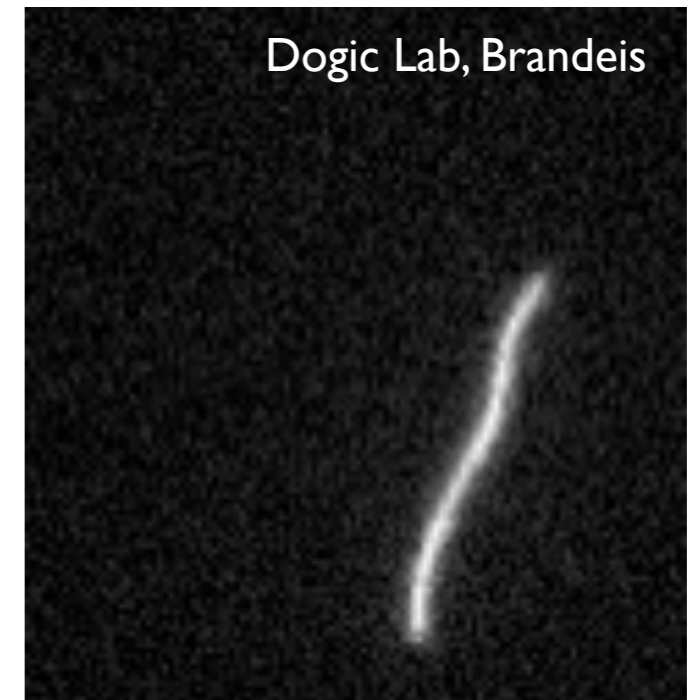
photo:
Philipp Khuc- Trong

Microtubuli network in *Drosophila* embryo

Polymers & filaments

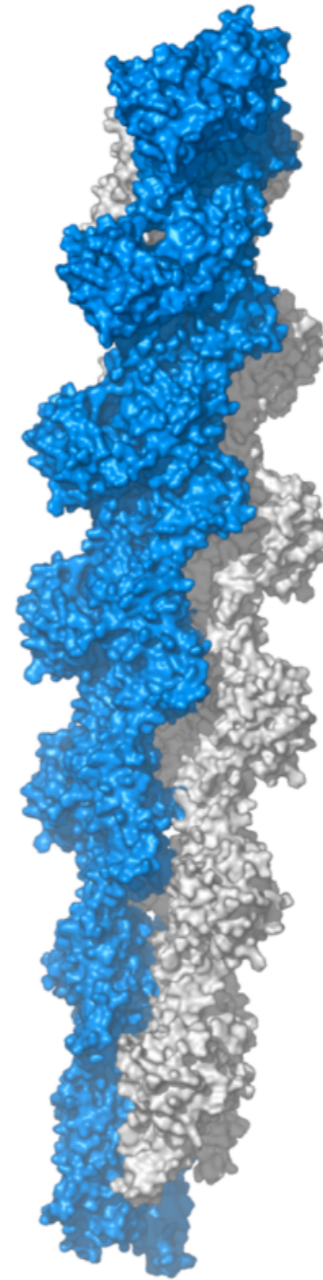


Drosophila oocyte



Physical parameters
(e.g. bending rigidity)
from fluctuation
analysis

Actin in 2D

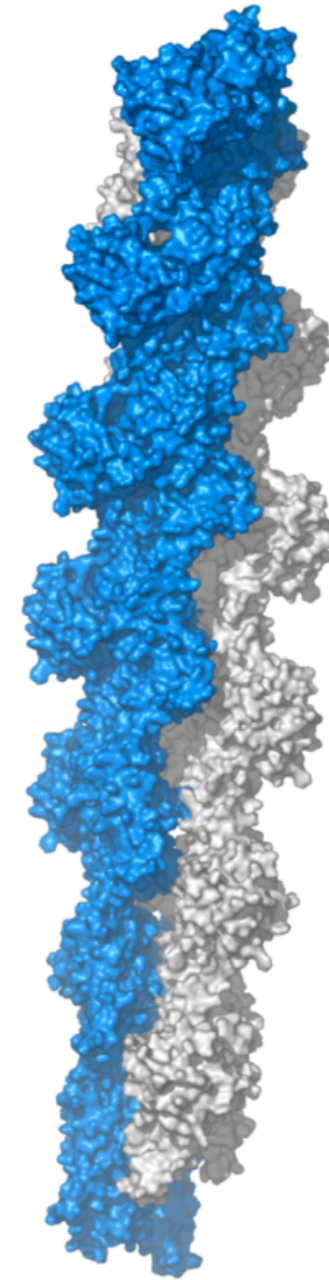


F-Actin

helical
filament

Dogic Lab (Brandeis)

Actin in 2D

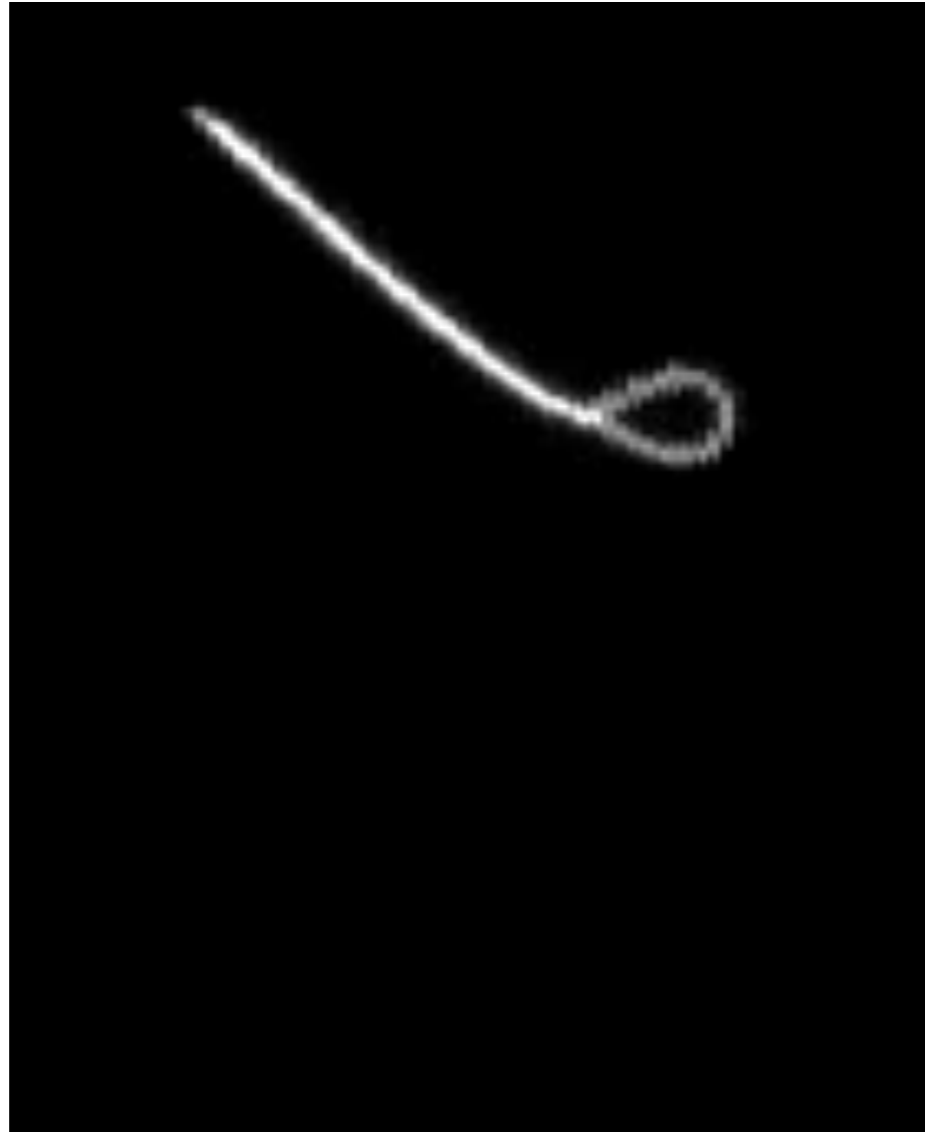


F-Actin

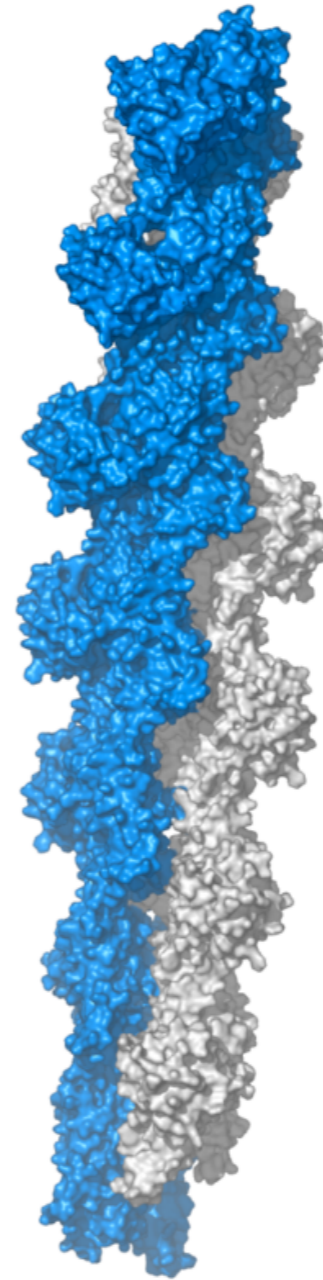
helical
filament

Dogic Lab (Brandeis)

Actin in 2D



with attractive solvent



F-Actin

helical
filament

Dogic Lab (Brandeis)

Actin in flow

PRL 108, 038103 (2012)

PHYSICAL REVIEW LETTERS

week ending
20 JANUARY 2012

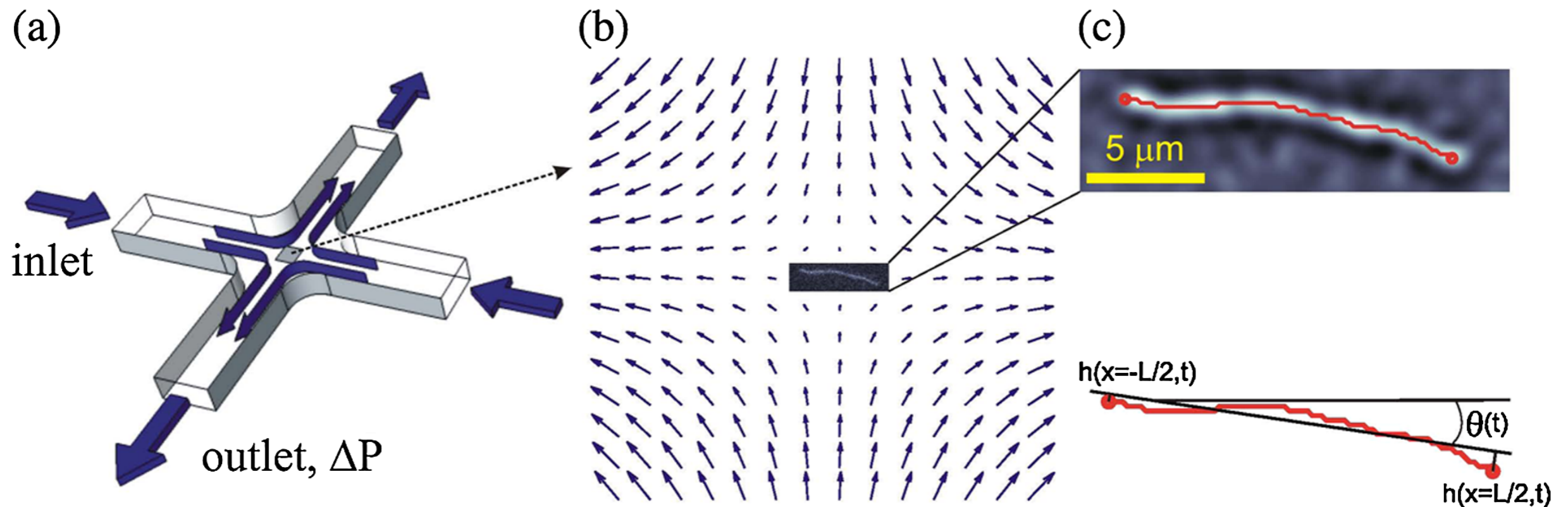
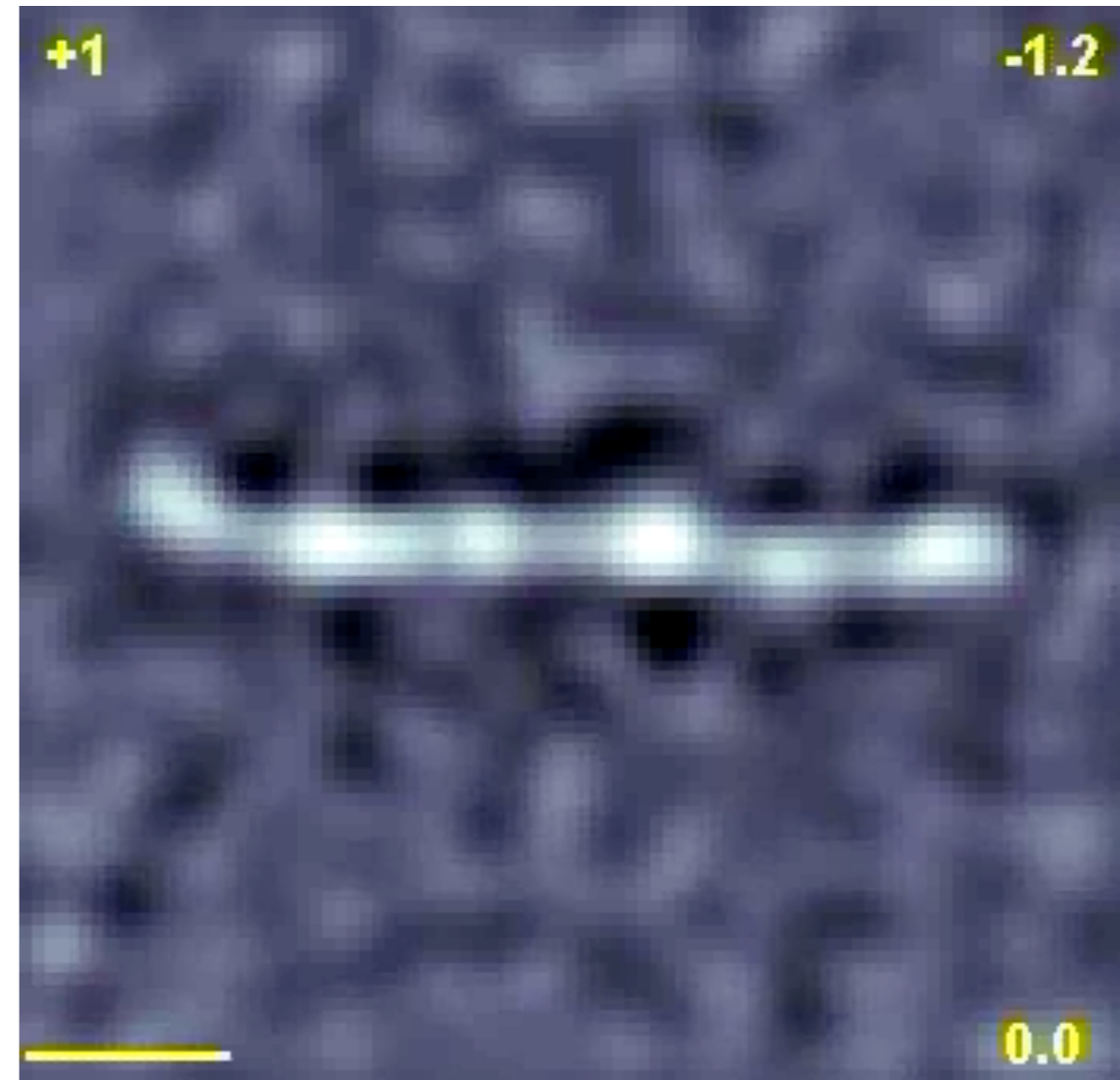
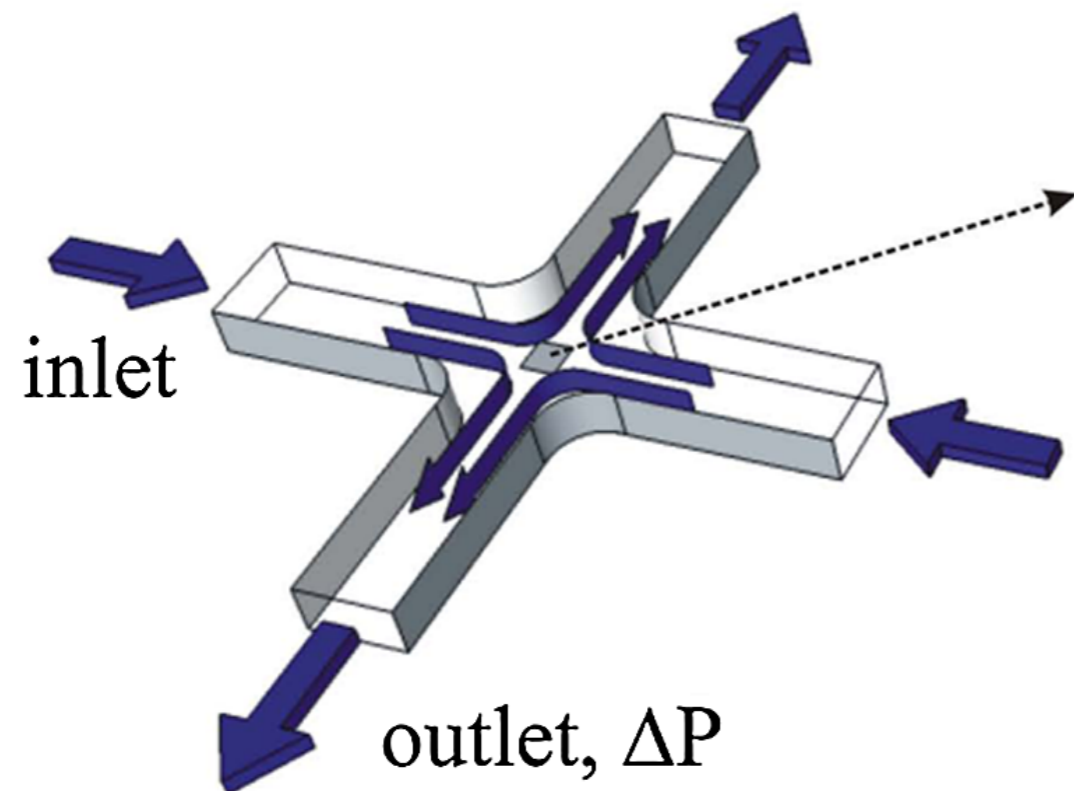


FIG. 1 (color online). Experimental setup. (a) Microfluidic cross-flow geometry controlled by a pressure difference ΔP between inlet and outlet branches. (b) Close-up of the velocity field near the stagnation point, showing a typical actin filament. (c) Raw contour (red) of an actin filament and definition of geometric quantities used in the analysis.

Kantsler & Goldstein (2012) PRL

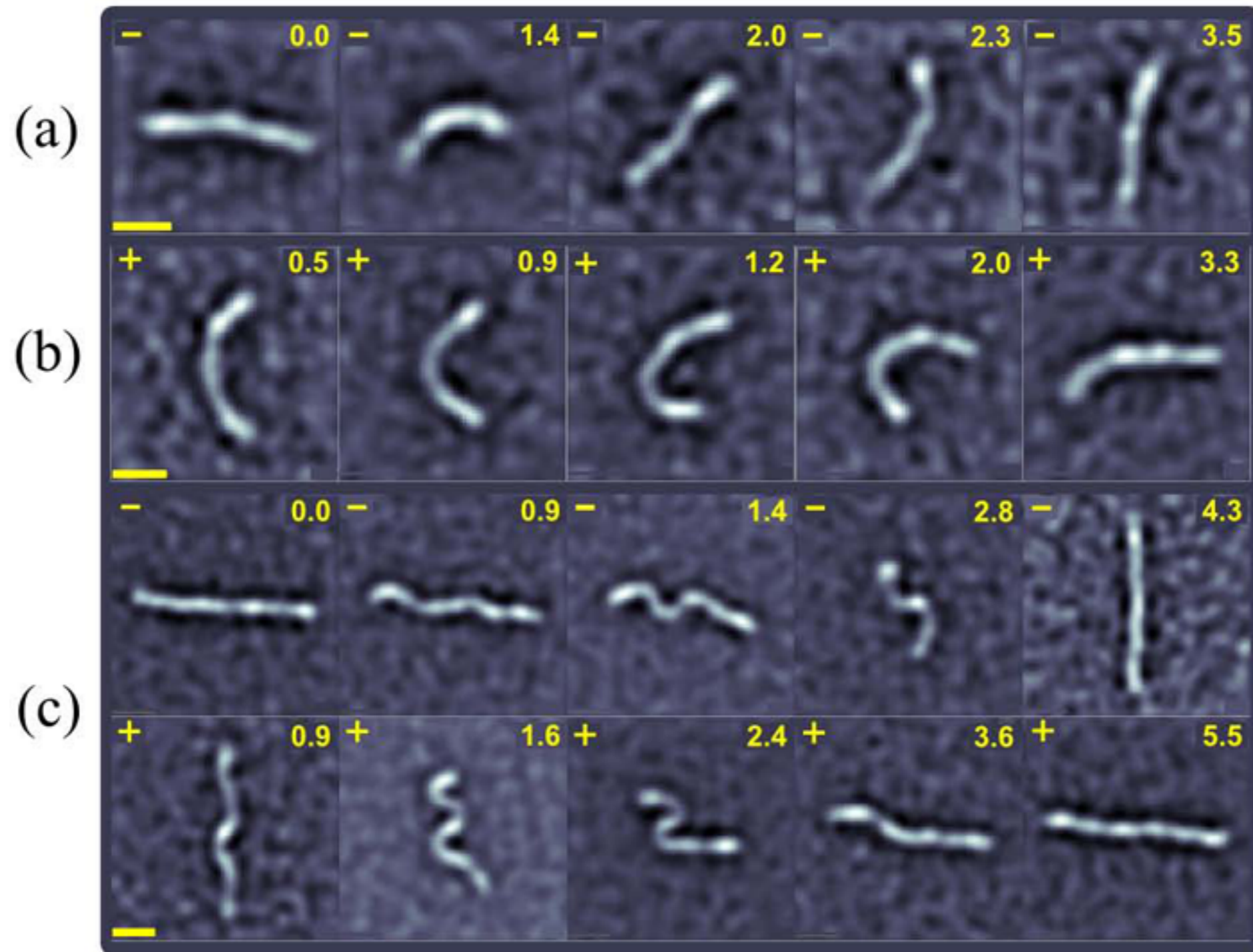
Actin in flow

(a)



Kantsler & Goldstein (2012) PRL

Actin in flow



Kantsler & Goldstein (2012) PRL

Theory

$$\mathcal{E} = \frac{1}{2} \int_{-L/2}^{L/2} dx \{ A h_{xx}^2 + \sigma(x) h_x^2 \}, \quad (1)$$

where subscripts indicate differentiation. The *nonuniform* tension induced by the flow [19],

$$\sigma(x) = \frac{2\pi\mu\dot{\gamma}}{\ln(1/\epsilon^2 e)} (L^2/4 - x^2), \quad (2)$$

Theory

of eigenfunctions $W^{(n)}$ (and eigenvalues λ_n) with boundary conditions $W_{xx}(\pm L/2) = W_{xxx}(\pm L/2) = 0$ [3,21]. Under the convenient rescaling $\xi = \pi x/L$, these obey

$$W_{4\xi}^{(n)} - \Sigma \partial_{\xi} [(\pi^2/4 - \xi^2) W_{\xi}^{(n)}] = \Lambda_n W^{(n)}. \quad (3)$$

The eigenvalues $\Lambda_n = L^4 \lambda_n / \pi^4 A$ are functions of [22]

$$\Sigma = \frac{2\mu \dot{\gamma} L^4}{\pi^3 A \ln(1/\epsilon^2 e)}. \quad (4)$$

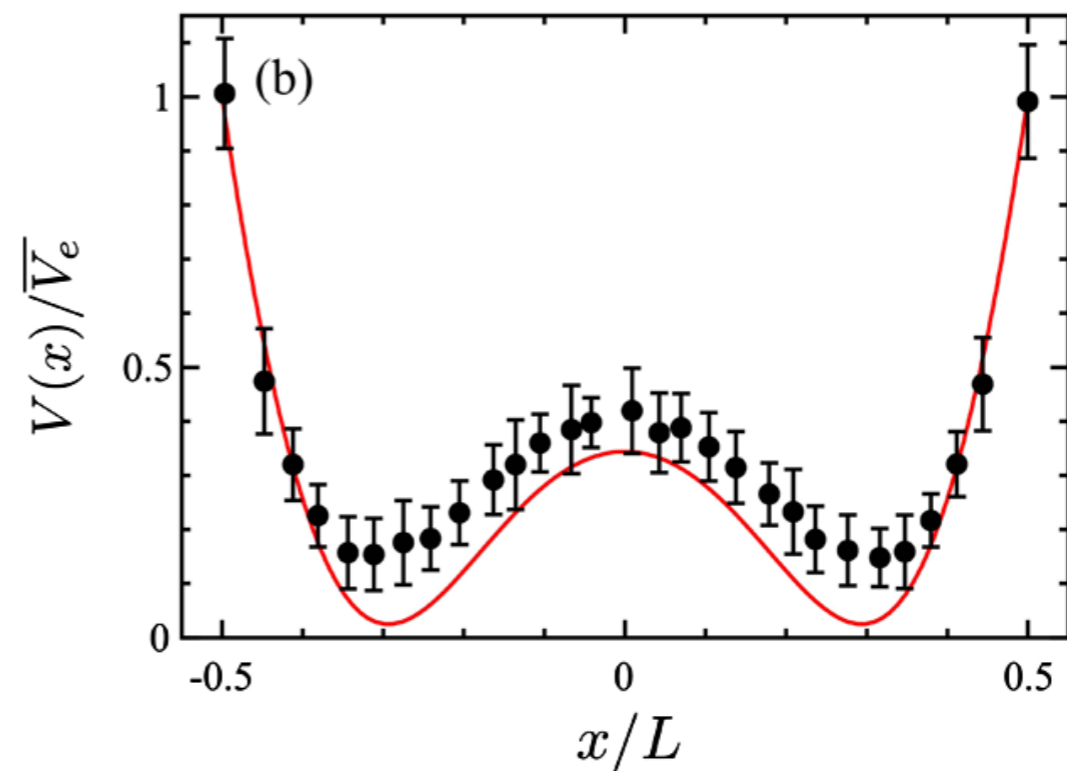
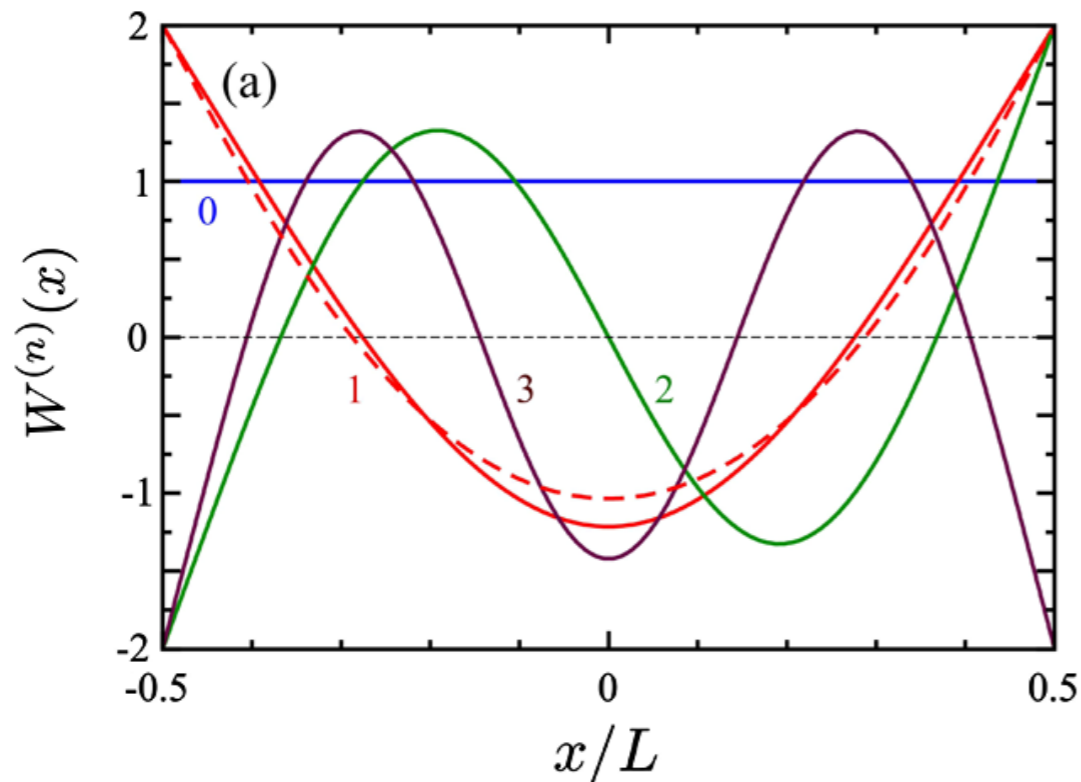
When $\Sigma = 0$, the $W^{(n)}$ are eigenfunctions of the one-dimensional biharmonic equation

$$W_{\Sigma=0} = A \sin kx + B \sinh kx + D \cos kx + E \cosh kx. \quad (5)$$

Theory vs. experiment

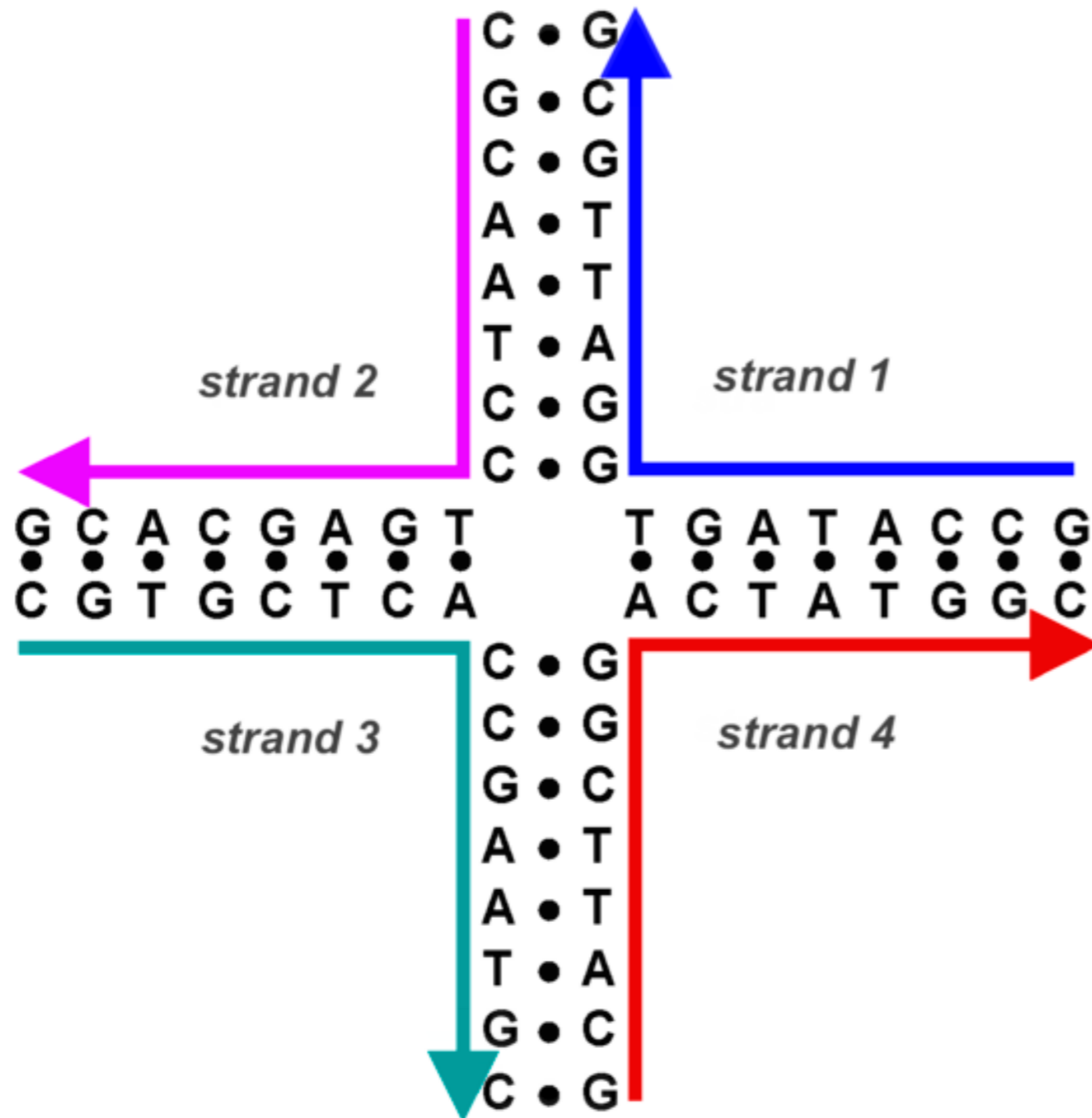
(and we assume they are normalized). Equipartition then yields $\langle a_m a_n \rangle = \delta_{mn} L^4 / \pi^4 \ell_p \Lambda_n$, and the local variance $V(x) = \langle [h(x) - \bar{h}]^2 \rangle$ is

$$V(x; \Sigma) = \frac{L^3}{\ell_p \pi^4} \sum_{n=1}^{\infty} \frac{W^{(n)}(x)^2}{\Lambda_n(\Sigma)}.$$



**Bio-technology
&
Soft Active Materials**

DNA Origami - principle



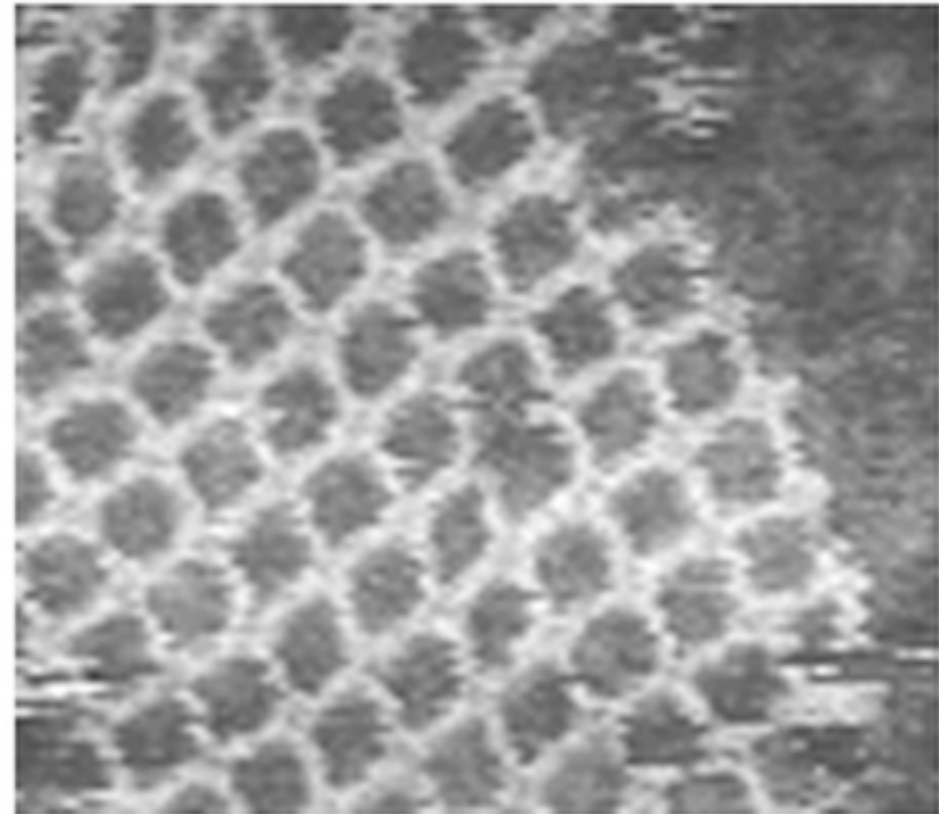
source: wiki

DNA Origami - principle

A



B

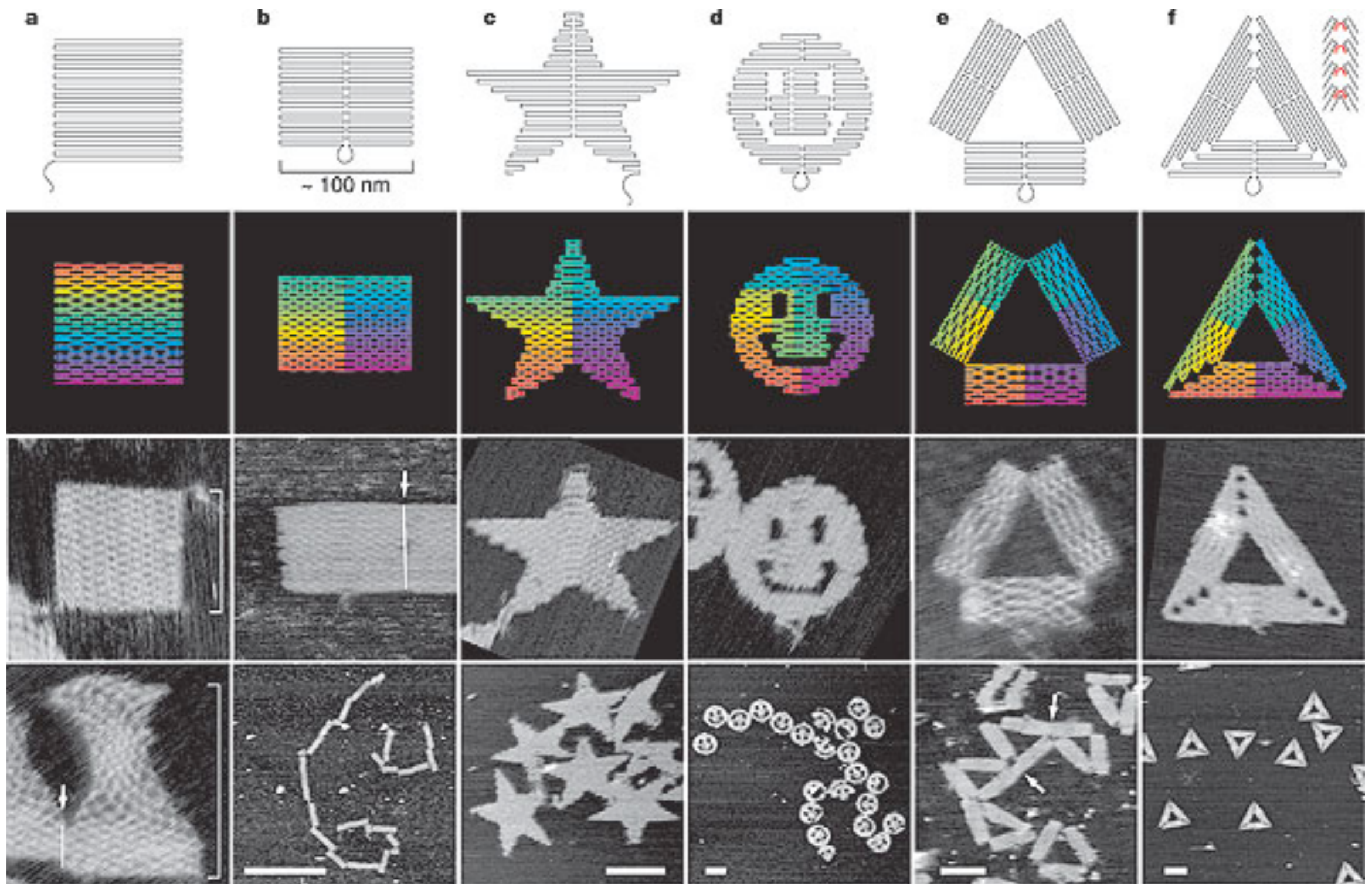


100 nm



Strong M: *Protein Nanomachines*. PLoS Biol 2/3/2004: e73

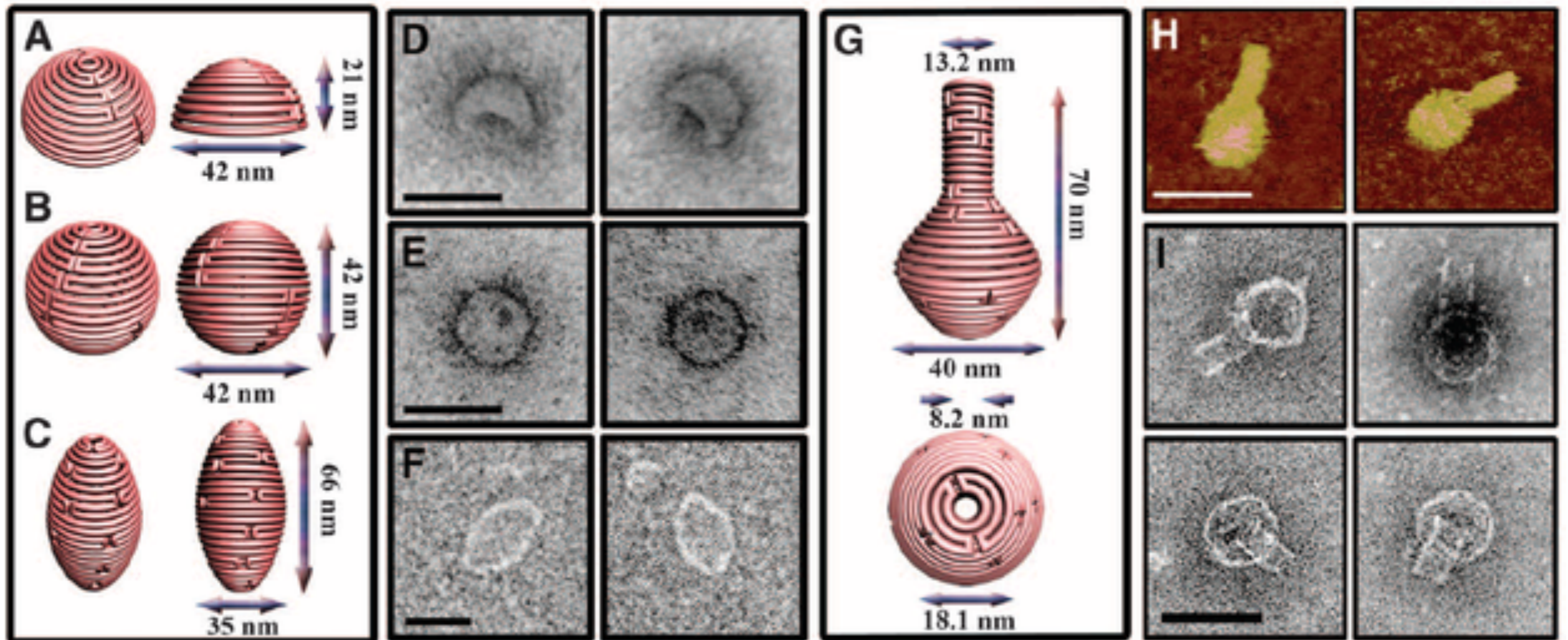
DNA Origami - 2D



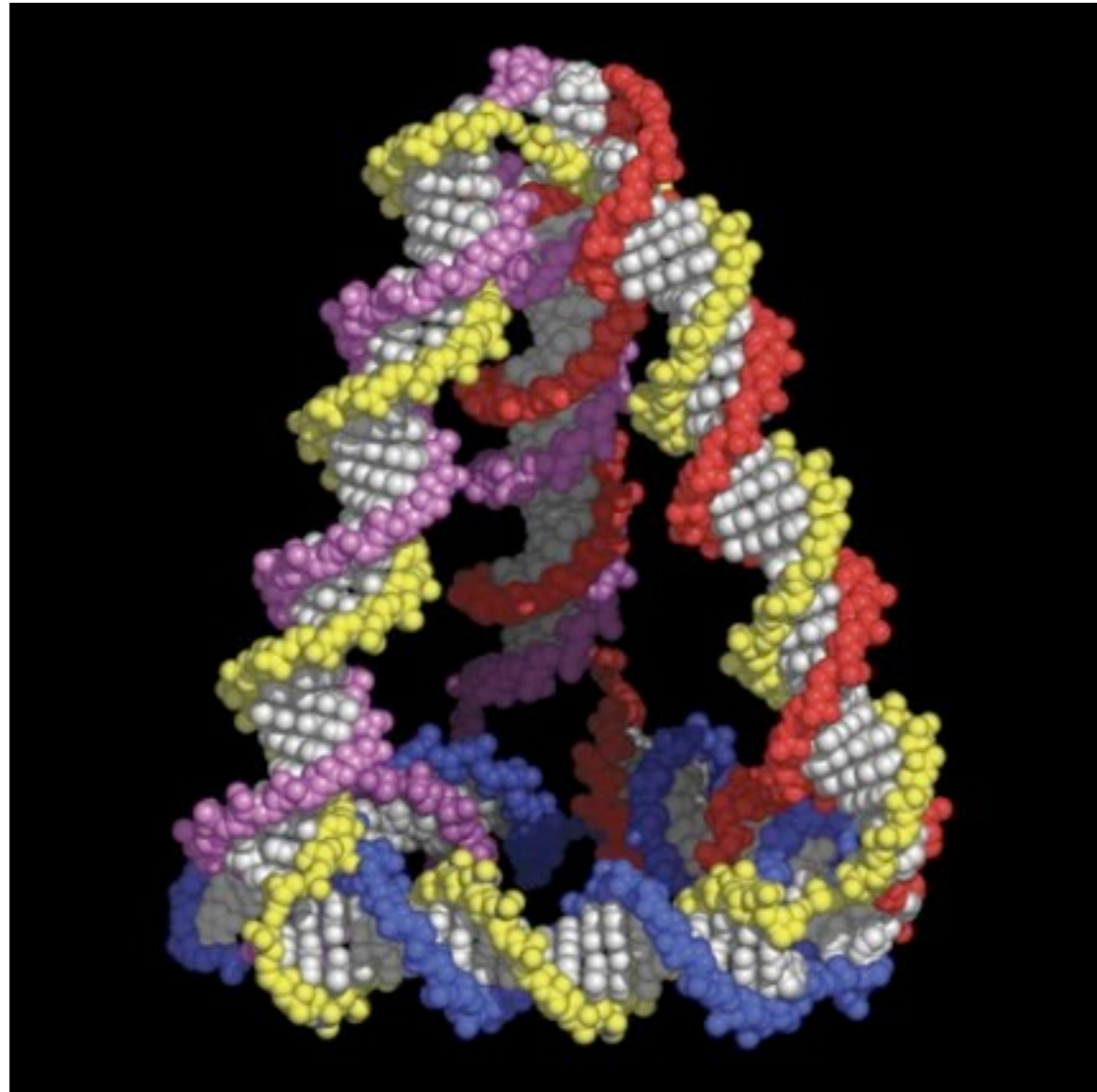
http://www.nature.com/scitable/blog/bio2.0/dna_origami

dunkel@math.mit.edu

DNA Origami - 3D



DNA polyhedra



edge \sim 10nm

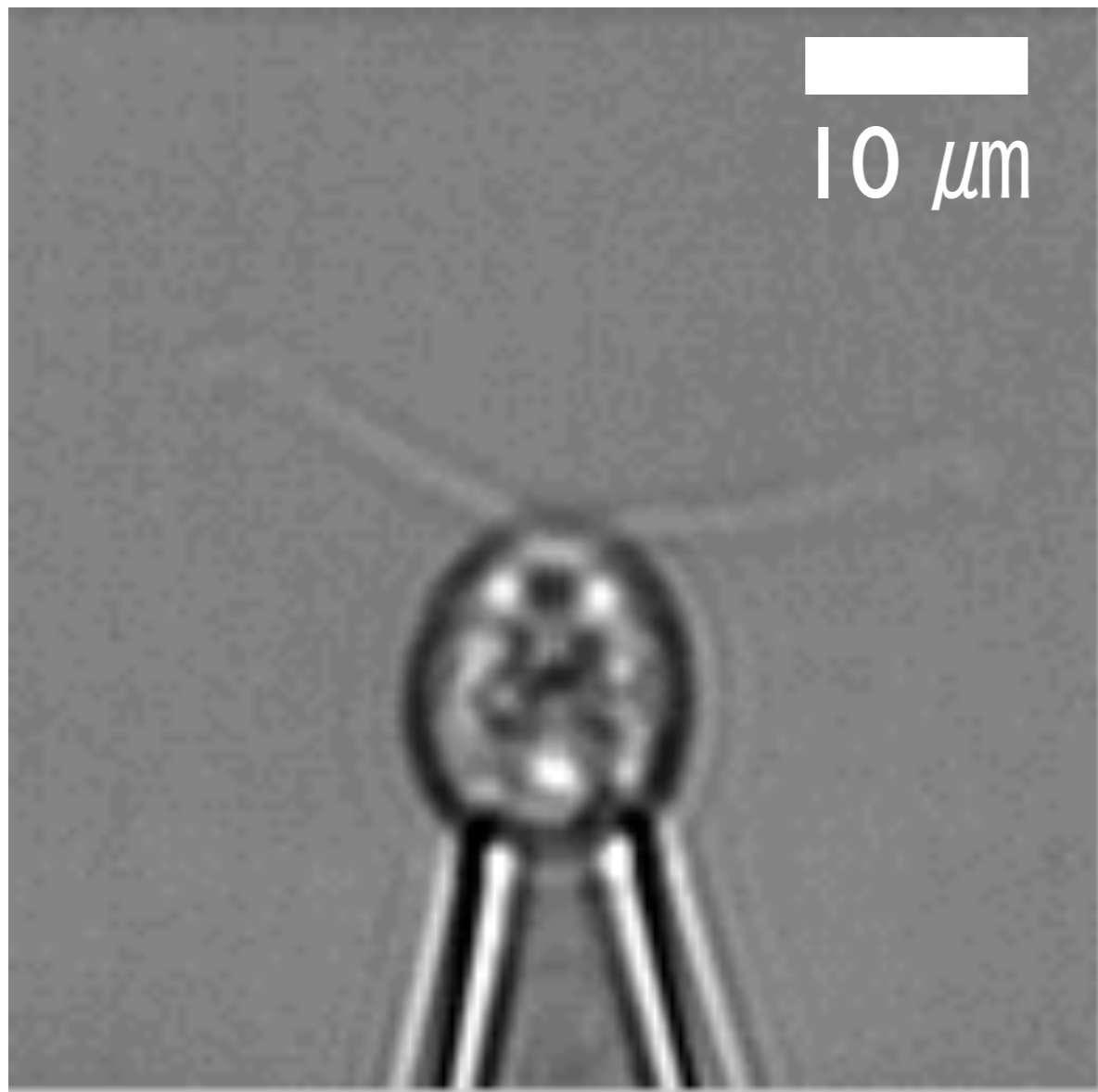
A rigid tetrahedron formed by self-assembly from DNA,
figure from [Goodman et al, Science 310 p1661 \(2005\)](#)

Computation

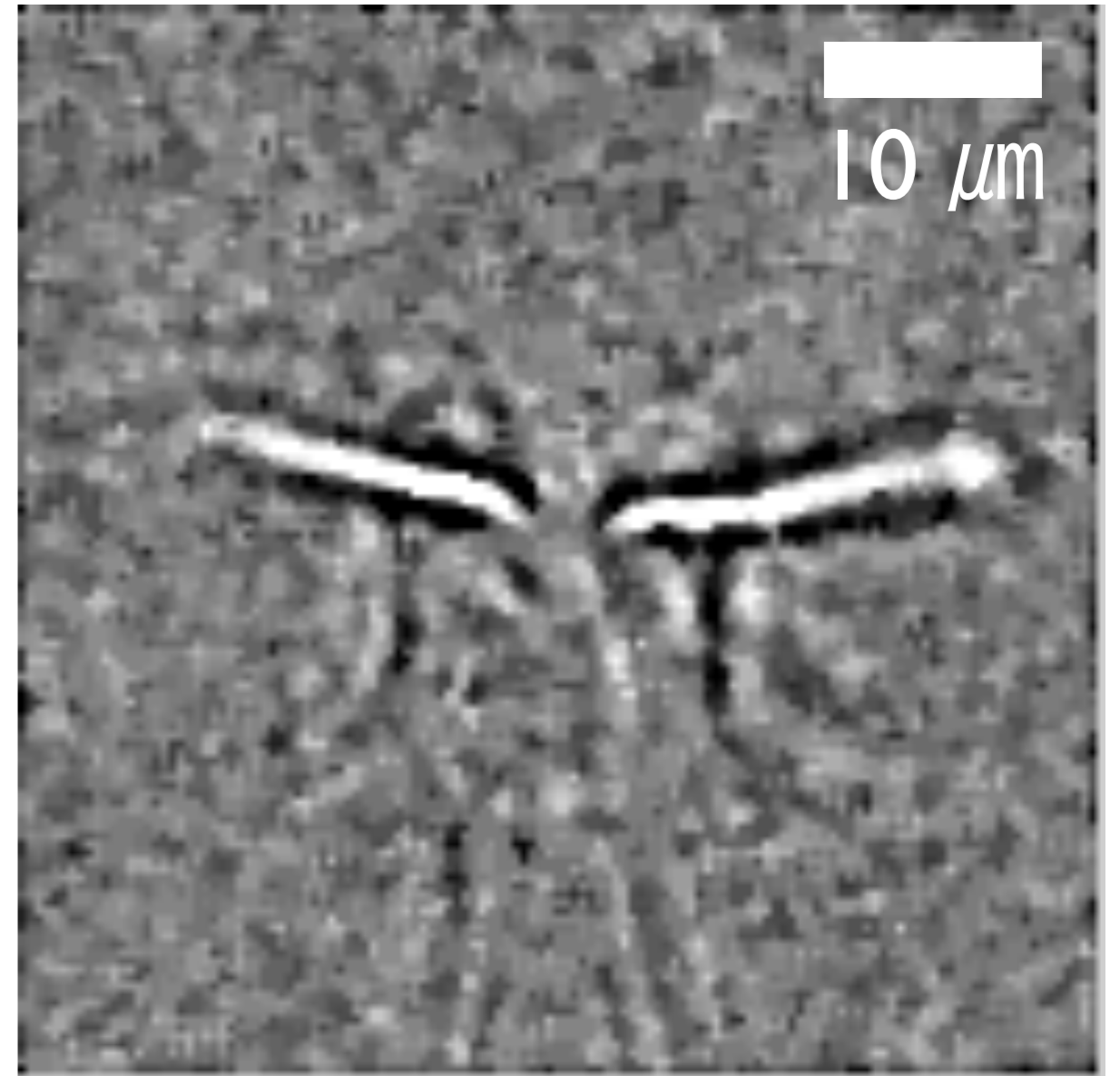
Mark Bathe, MIT

<http://lcbb.mit.edu/software/index.html>

Artificial cilia

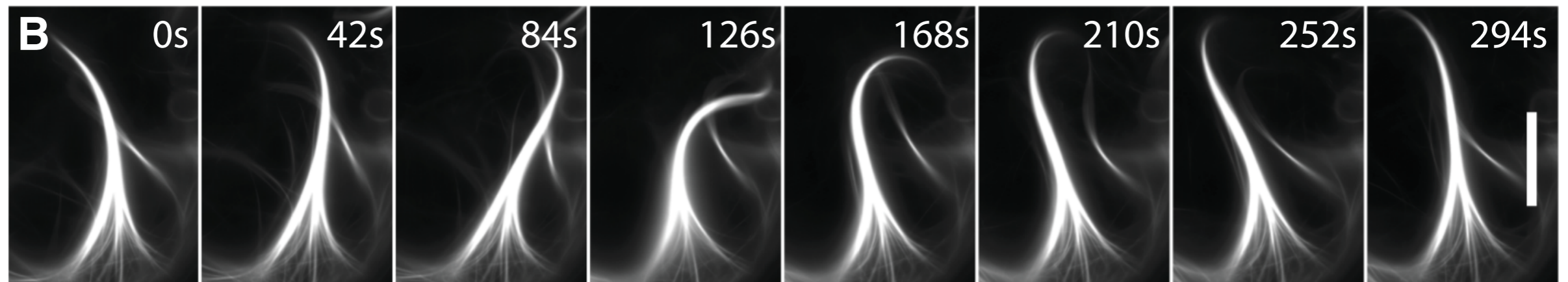
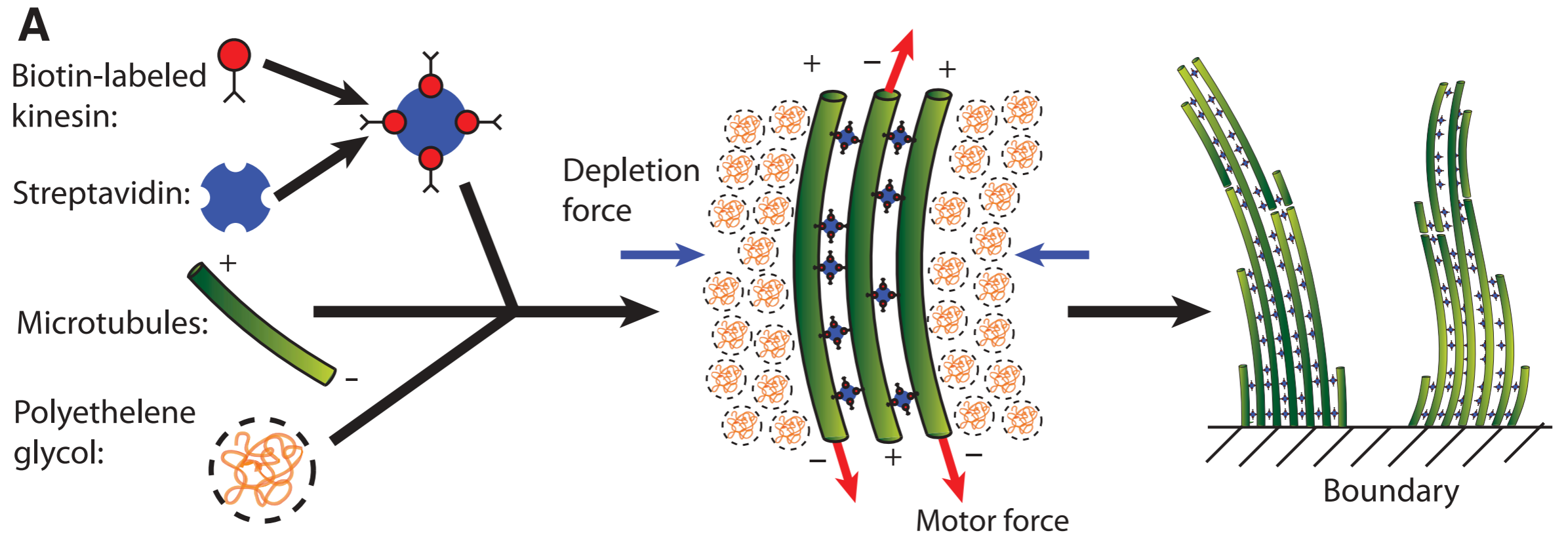


~ 50 beats / sec



speed ~100 μm/s

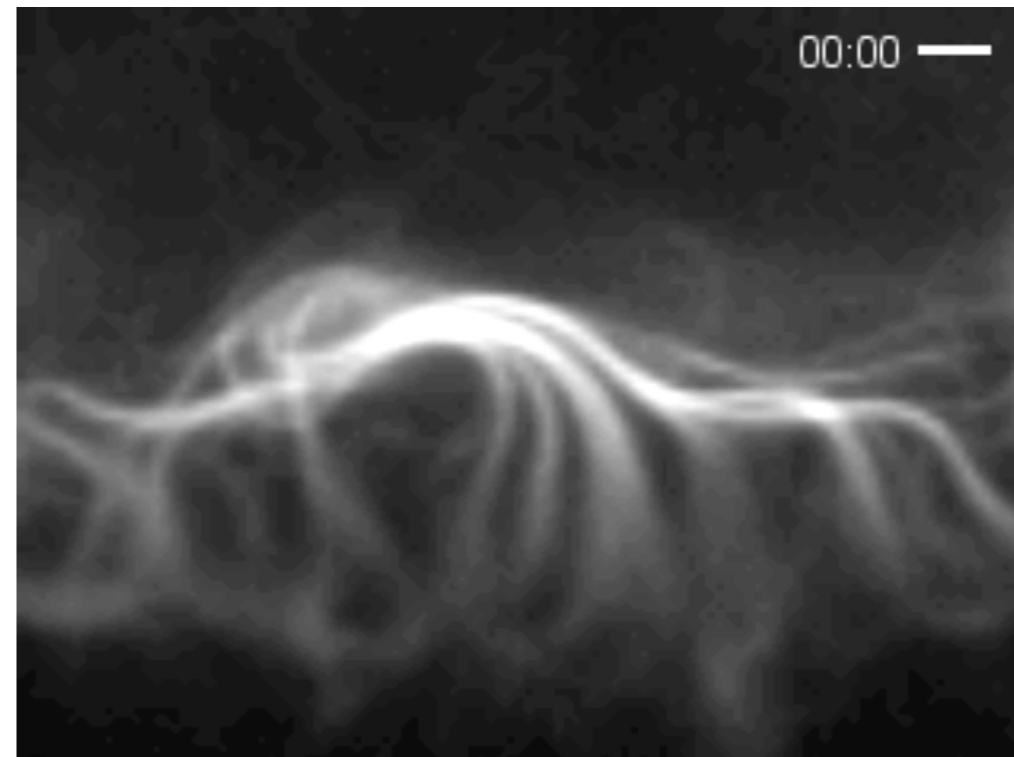
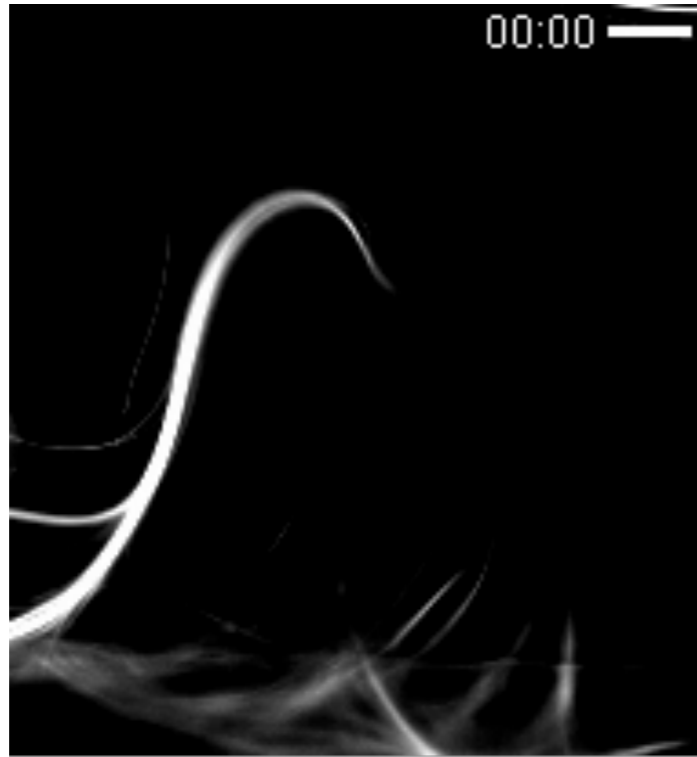
Artificial cilia



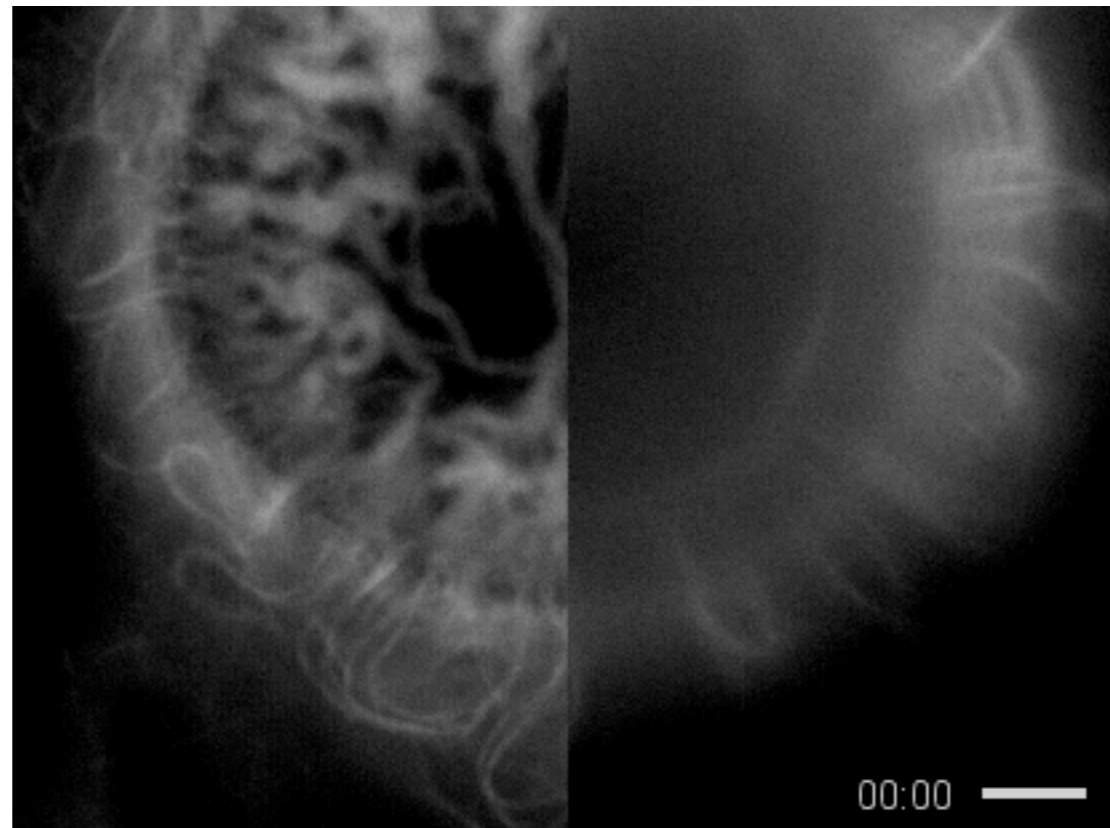
Dogic Lab (Brandeis)

Science 2011

Artificial cilia



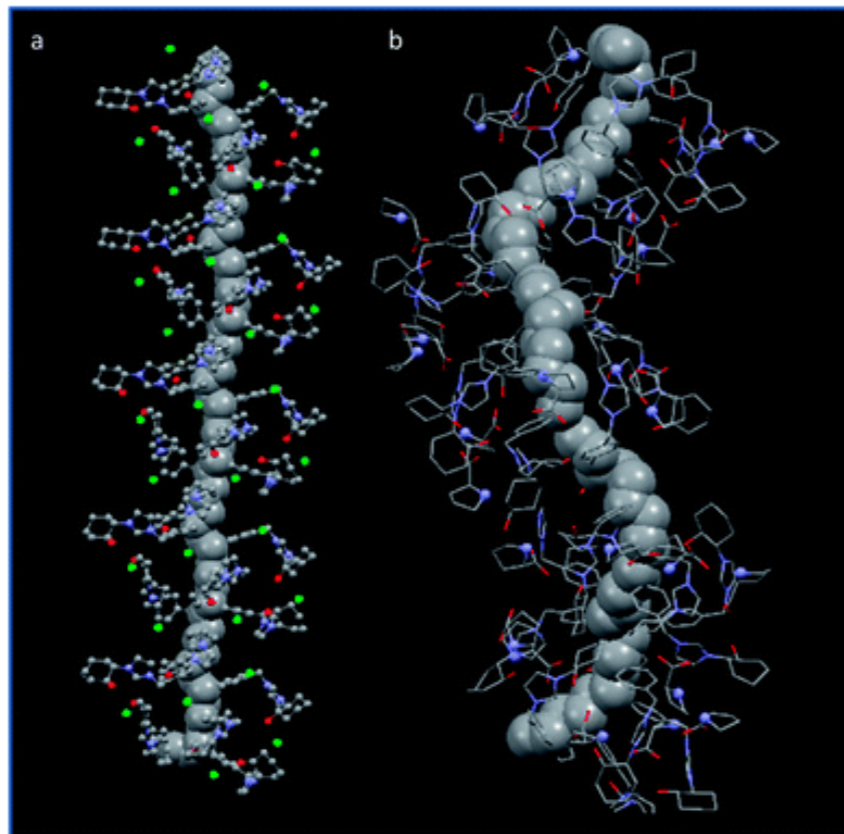
Dogic Lab
(Brandeis)



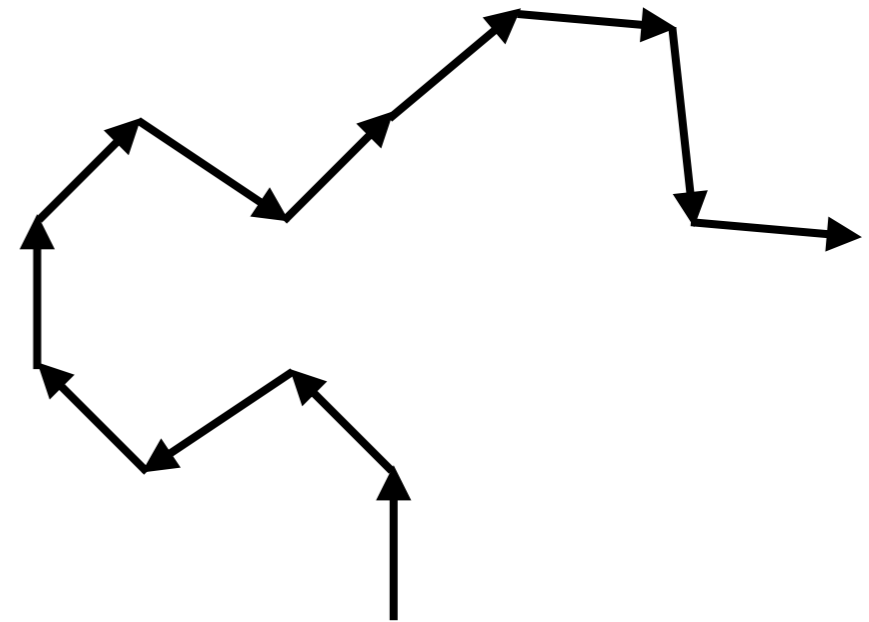
Science 2011

Basic polymer models

Karjalainen et al (2014) Polym Chem



<http://dx.doi.org/10.1039/1759-9962/2010>



2.1 Persistent random walks

2.1.1 von Mises-Fisher (vMF) distribution

The PDF of the vMF distribution on the unit sphere $\mathbf{n} \in \mathbb{S}$ reads

$$f(\mathbf{n}|\boldsymbol{\mu}) = C_2 e^{\kappa \mathbf{n} \cdot \boldsymbol{\mu}}. \quad (2.1)$$

The parameter $\boldsymbol{\mu} \in \mathbb{S}$ determines the mean direction and κ the spread, with $\kappa = 0$ corresponding to a uniform distribution and $\kappa \rightarrow \infty$ to a δ -distribution at $\mathbf{n} = \boldsymbol{\mu}$. Assuming w.l.o.g. $\boldsymbol{\mu} = (0, 0, 1)$ and using spherical coordinates $\mathbf{n} = (\cos \phi \sin \theta, \sin \phi \sin \theta, \cos \theta)$ with $(\phi, \theta) \in [0, 2\pi) \times [0, \pi]$, the normalization constant C_2 can be computed from

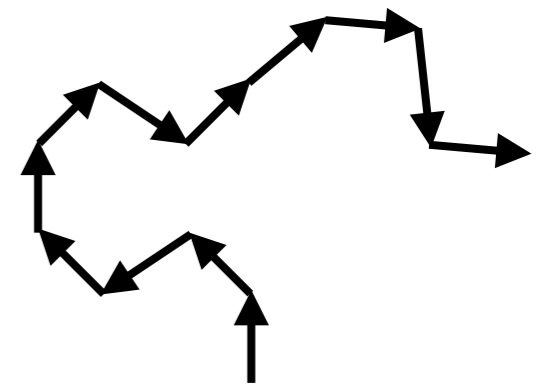
$$\begin{aligned} 1 &= C_2 \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta f(\mathbf{n}|\boldsymbol{\mu}) \\ &= C_2 \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta e^{\kappa \cos \theta} \\ &= C_2 \frac{4\pi \sinh \kappa}{\kappa}, \end{aligned} \quad (2.2)$$

yielding

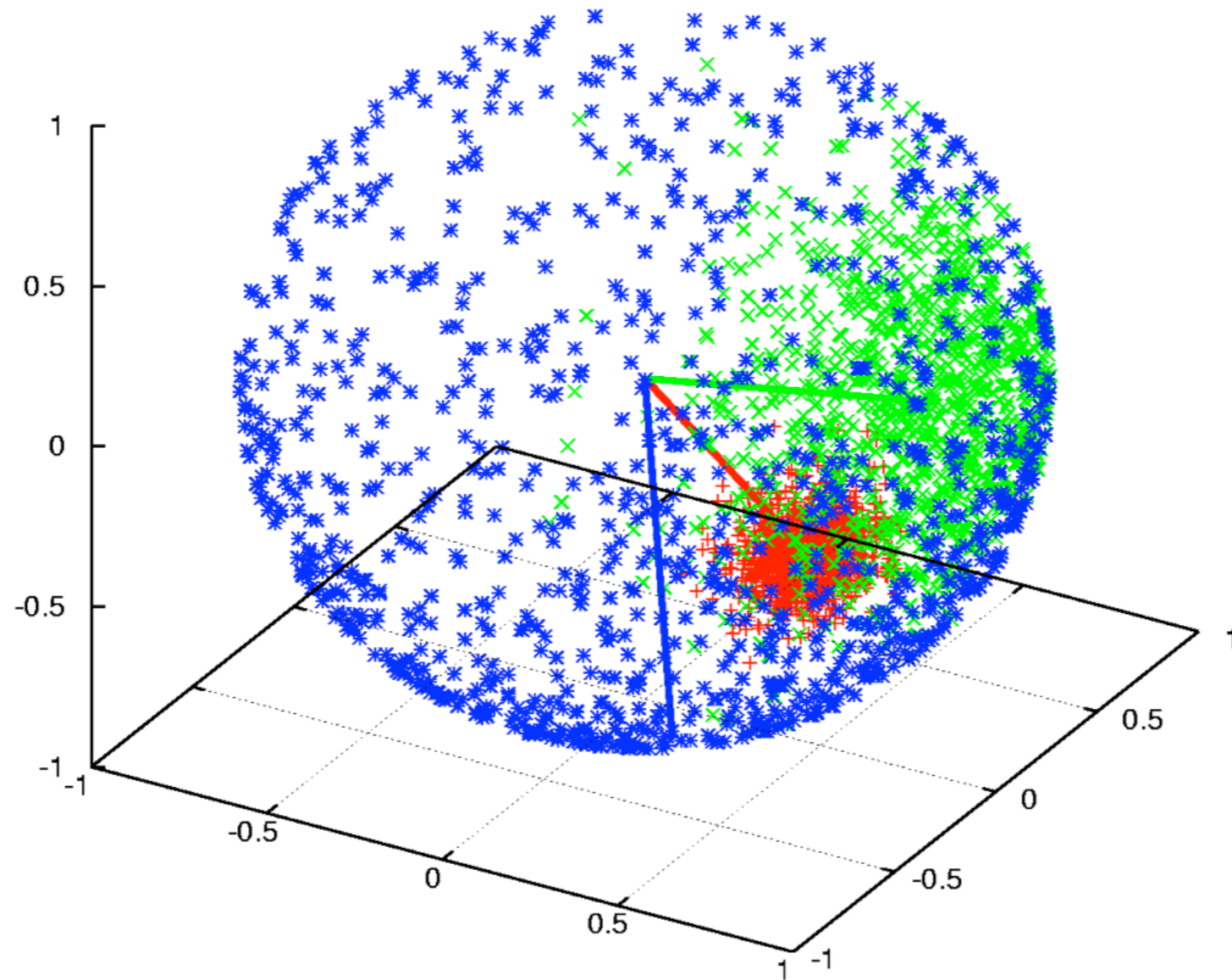
$$C_2 = \frac{\kappa}{4\pi \sinh \kappa}. \quad (2.3)$$

Similarly, one finds for the mean

$$\mathbb{E}[\mathbf{n}|\boldsymbol{\mu}] = C_2 \int d\mathbf{n} \mathbf{n} e^{\kappa \mathbf{n} \cdot \boldsymbol{\mu}} = \left(\frac{1}{\tanh \kappa} - \frac{1}{\kappa} \right) \boldsymbol{\mu} =: \sigma \boldsymbol{\mu}, \quad (2.4a)$$



von Mises-Fisher distribution



$$\kappa = 1$$

$$\kappa = 10$$

$$\kappa = 100$$

arrows = mean direction

2.1.1 von Mises-Fisher (vMF) distribution

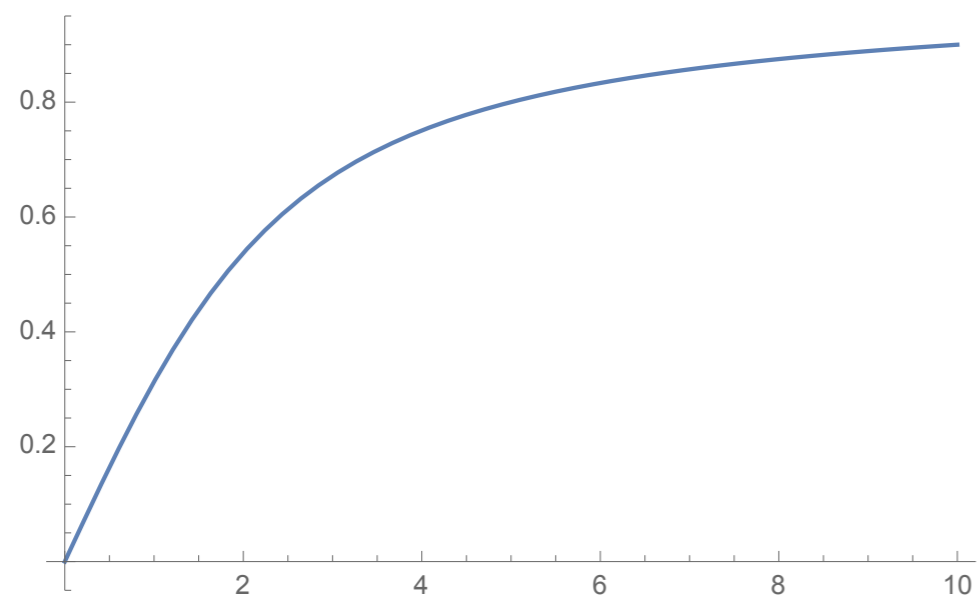
$$f(\mathbf{n}|\boldsymbol{\mu}) = C_2 e^{\kappa \mathbf{n} \cdot \boldsymbol{\mu}}. \quad (2.1)$$

$$\mathbb{E}[\mathbf{n}|\boldsymbol{\mu}] = C_2 \int d\mathbf{n} \mathbf{n} e^{\kappa \mathbf{n} \cdot \boldsymbol{\mu}} = \left(\frac{1}{\tanh \kappa} - \frac{1}{\kappa} \right) \boldsymbol{\mu} =: \sigma \boldsymbol{\mu}, \quad (2.4a)$$

where the scale-factor $\sigma(\kappa)$ exhibits the following limiting behaviors

$$\lim_{\kappa \rightarrow 0} \sigma(\kappa) = 0, \quad (2.4b)$$

$$\lim_{\kappa \rightarrow \infty} \sigma(\kappa) = 1. \quad (2.4c)$$



2.1.2 vMF polymer model

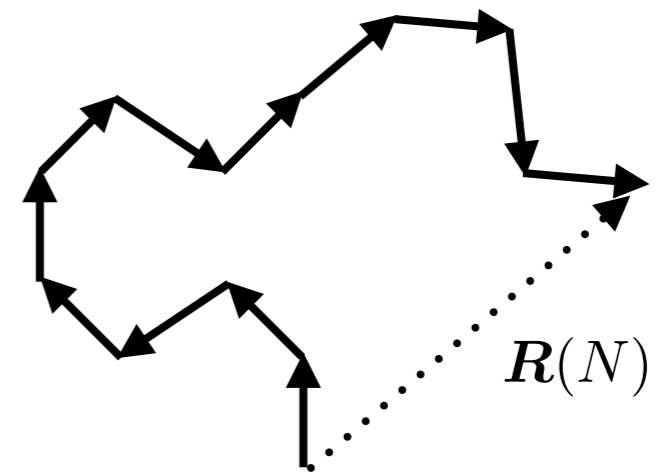
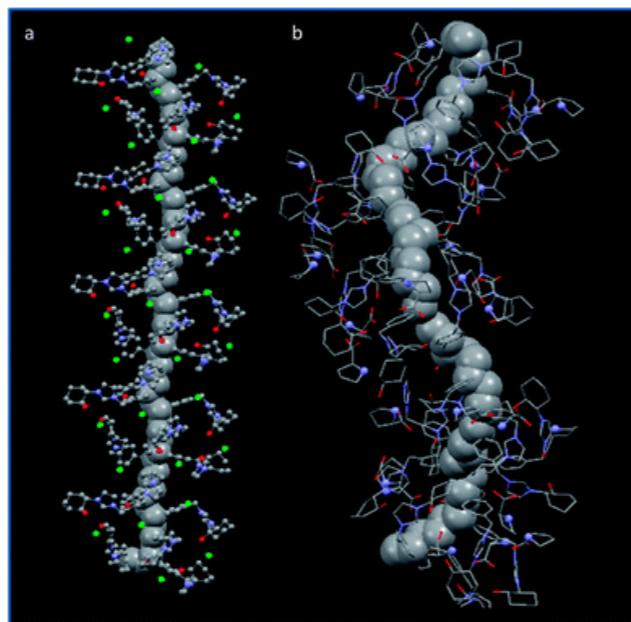
Consider an idealized polymer consisting of $i = 1, \dots, N$ segments of length λ . Each segment has an orientation $\boldsymbol{\mu}_i$, so that the vector connecting the two polymer ends is given by

$$\mathbf{R}(N) = \sum_{i=1}^N \mathbf{R}_i = \lambda \sum_{i=1}^N \boldsymbol{\mu}_i. \quad (2.5)$$

The total length of the polymer is $L = N\lambda$ and w.l.o.g. we choose $\mathbf{R}(0)$ and $\boldsymbol{\mu}_1 = (0, 0, 1)$. We assume that the conditional PDF of $\boldsymbol{\mu}_i$ for a given $\boldsymbol{\mu}_{i-1}$, is a vMF-distribution with spread parameter κ ,

$$f(\boldsymbol{\mu}_i | \boldsymbol{\mu}_{i-1}) = C_2 e^{\kappa \boldsymbol{\mu}_i \cdot \boldsymbol{\mu}_{i-1}}. \quad (2.6)$$

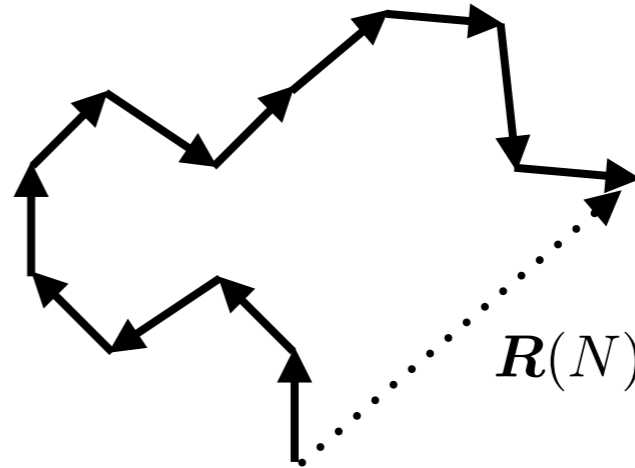
Karjalainen et al (2014) Polym Chem



<http://dx.doi.org/10.1039/1759-9962/2010>

dunkel@math.mit.edu

$$\mathbf{R}(N) = \sum_{i=1}^N \mathbf{R}_i = \lambda \sum_{i=1}^N \boldsymbol{\mu}_i.$$



We would like to compute correlation functions and statistical moments of $\mathbf{R}(N)$ in the limit of large N . Of particular interest are the mean end-position

$$\mathbb{E}[\mathbf{R}(N)|\boldsymbol{\mu}_1] = \lambda \sum_{n=1}^N \mathbb{E}[\boldsymbol{\mu}_n|\boldsymbol{\mu}_1], \quad (2.7a)$$

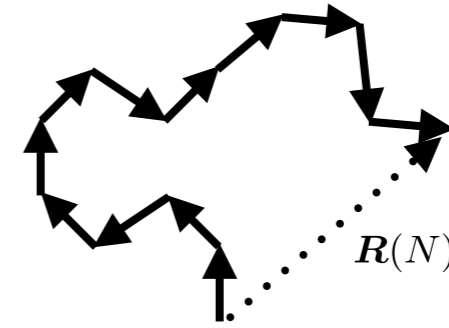
the squared end-to-end distance

$$\mathcal{D}(N) = \mathbb{E}[\mathbf{R}(N) \cdot \mathbf{R}(N)], \quad (2.7b)$$

and the excursion PDF

$$p_N(\mathbf{r}) = \mathbb{E}[\delta(\mathbf{r} - \mathbf{R}(N))]. \quad (2.7c)$$

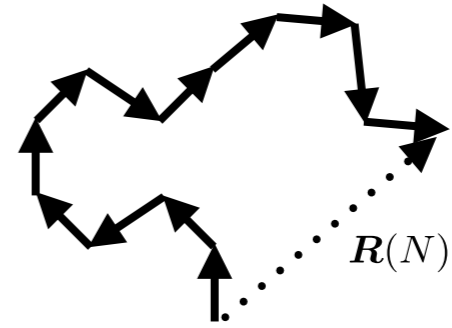
$$\mathbb{E}[\mathbf{R}(N)|\boldsymbol{\mu}_1] = \lambda \sum_{n=1}^N \mathbb{E}[\boldsymbol{\mu}_n|\boldsymbol{\mu}_1],$$



Mean end-position and persistence length

To compute the mean end-position $\mathbb{E}[\mathbf{R}(N)|\boldsymbol{\mu}_1]$ for a given initial condition $\boldsymbol{\mu}_1$, let us first note that the conditional expectation value $\mathbb{E}[\boldsymbol{\mu}_n|\boldsymbol{\mu}_1]$ can be computed as

$$\begin{aligned} \mathbb{E}[\boldsymbol{\mu}_n|\boldsymbol{\mu}_1] &= C_2^{m-1} \int \boldsymbol{\mu}_n e^{\kappa \sum_{i=2}^N \boldsymbol{\mu}_i \cdot \boldsymbol{\mu}_{i-1}} \prod_{i=2}^n d\boldsymbol{\mu}_i \\ &= \sigma C_2^{m-2} \int \boldsymbol{\mu}_{n-1} e^{\kappa \sum_{i=2}^{n-1} \boldsymbol{\mu}_i \cdot \boldsymbol{\mu}_{i-1}} \prod_{i=2}^{n-1} d\boldsymbol{\mu}_i \\ &\dots \\ &= \sigma^{n-1} \boldsymbol{\mu}_1, \end{aligned} \tag{2.8}$$



Mean end-position and persistence length

$$\mathbb{E}[\mathbf{R}(N)|\boldsymbol{\mu}_1] = \lambda \sum_{n=1}^N \sigma^{n-1} \boldsymbol{\mu}_1 = \lambda \sum_{n=0}^{N-1} \sigma^n \boldsymbol{\mu}_1 = \lambda \frac{1 - \sigma^N}{1 - \sigma} \boldsymbol{\mu}_1$$

In the limit case of a uniform distribution, $\kappa \rightarrow 0$, we find at fixed N

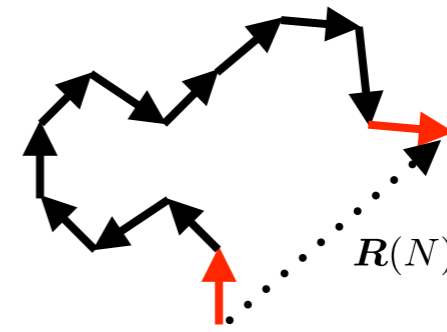
$$\mathbb{E}[\mathbf{R}(N)|\boldsymbol{\mu}_1] = \lambda \boldsymbol{\mu}_1 \quad (2.10a)$$

whereas for an infinitely stiff polymer with $\kappa \rightarrow \infty$

$$\mathbb{E}[\mathbf{R}(N)|\boldsymbol{\mu}_1] = \lambda N \boldsymbol{\mu}_1, \quad (2.10b)$$

illustrating that the vMF-model interpolates between undirected random walking and ballistic motion.

Mean end-position and persistence length L_P

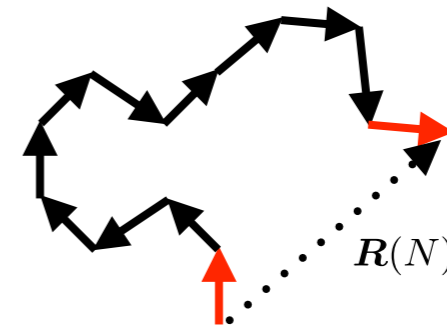


$$\langle \cos \theta_N \rangle \equiv \mathbb{E}[\boldsymbol{\mu}_N \cdot \boldsymbol{\mu}_1] \simeq e^{-L/L_P} \quad (2.11)$$

for large polymer length $L = N\lambda$. Noting that

$$\mathbb{E}[\boldsymbol{\mu}_N \cdot \boldsymbol{\mu}_1] = \mathbb{E}[\boldsymbol{\mu}_N | \boldsymbol{\mu}_1] \cdot \boldsymbol{\mu}_1, \quad (2.12)$$

Mean end-position and persistence length L_P



$$\langle \cos \theta_N \rangle \equiv \mathbb{E}[\boldsymbol{\mu}_N \cdot \boldsymbol{\mu}_1] \simeq e^{-L/L_P} \quad (2.11)$$

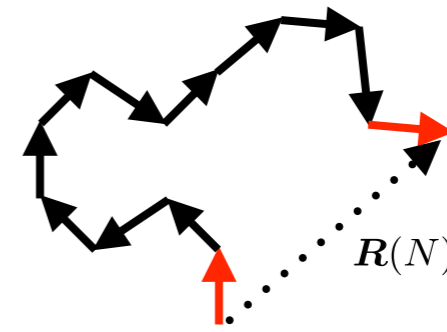
for large polymer length $L = N\lambda$. Noting that

$$\mathbb{E}[\boldsymbol{\mu}_N \cdot \boldsymbol{\mu}_1] = \mathbb{E}[\boldsymbol{\mu}_N | \boldsymbol{\mu}_1] \cdot \boldsymbol{\mu}_1, \quad (2.12)$$

we can obtain L_P from (2.8) by

$$\begin{aligned} \frac{1}{L_P} &= - \lim_{L \rightarrow \infty} \frac{1}{L} \ln \mathbb{E}[\boldsymbol{\mu}_N \cdot \boldsymbol{\mu}_1] \\ &= - \lim_{N \rightarrow \infty} \frac{1}{\lambda N} \ln \sigma^{N-1} \\ &= - \frac{1}{\lambda} \ln \sigma. \end{aligned} \quad (2.13)$$

Mean end-position and persistence length L_P



$$\langle \cos \theta_N \rangle \equiv \mathbb{E}[\boldsymbol{\mu}_N \cdot \boldsymbol{\mu}_1] \simeq e^{-L/L_P} \quad (2.11)$$

for large polymer length $L = N\lambda$. Noting that

$$\mathbb{E}[\boldsymbol{\mu}_N \cdot \boldsymbol{\mu}_1] = \mathbb{E}[\boldsymbol{\mu}_N | \boldsymbol{\mu}_1] \cdot \boldsymbol{\mu}_1, \quad (2.12)$$

we can obtain L_P from (2.8) by

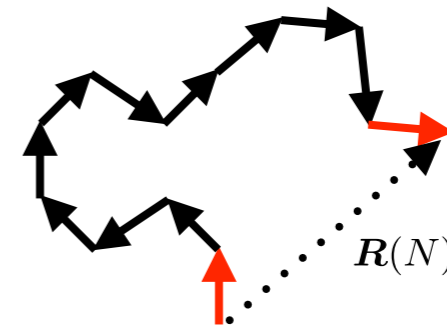
$$\begin{aligned} \frac{1}{L_P} &= - \lim_{L \rightarrow \infty} \frac{1}{L} \ln \mathbb{E}[\boldsymbol{\mu}_N \cdot \boldsymbol{\mu}_1] \\ &= - \lim_{N \rightarrow \infty} \frac{1}{\lambda N} \ln \sigma^{N-1} \\ &= - \frac{1}{\lambda} \ln \sigma. \end{aligned} \quad (2.13)$$

Inserting the explicit expression $\sigma(\kappa)$ from (2.4a), we find for $\kappa \ll 1$

$$L_P \simeq \frac{\lambda}{\ln(3/\kappa)}, \quad (2.14a)$$

whereas for $\kappa \gg 1$

$$L_P \simeq \lambda \kappa. \quad (2.14b)$$



Squared end-to-end distance

To compute the squared end-to-end distance

$$\mathcal{D}(N) = \mathbb{E}[\mathbf{R}(N) \cdot \mathbf{R}(N)] = \lambda^2 \sum_{i,j=1}^N \mathbb{E}[\boldsymbol{\mu}_i \cdot \boldsymbol{\mu}_j], \quad (2.15)$$

we may use that the orientation correlation is translation-invariant

$$\mathbb{E}[\boldsymbol{\mu}_i \cdot \boldsymbol{\mu}_j] = \sigma^{|i-j|}. \quad (2.16)$$

Computing the double sum (2.15), one obtains

$$\mathcal{D}(N) = \lambda^2 \frac{N - \sigma(2 - 2\sigma^N + \sigma N)}{(\sigma - 1)^2}, \quad (2.17)$$

and from this the limiting behaviors

$$\lim_{\kappa \rightarrow 0} \mathcal{D}(N) = \lim_{\sigma \rightarrow 0} \mathcal{D}(N) = \lambda^2 N, \quad (2.18a)$$

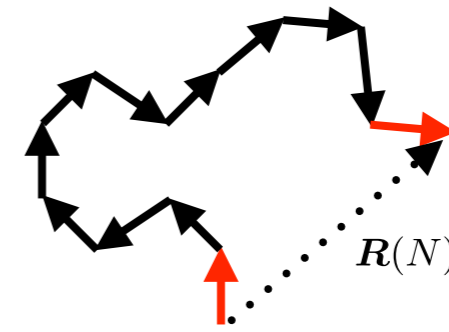
$$\lim_{\kappa \rightarrow \infty} \mathcal{D}(N) = \lim_{\sigma \rightarrow 1} \mathcal{D}(N) = \lambda^2 N^2, \quad (2.18b)$$

corresponding to normal diffusion and ballistic growth. Conversely, when keeping $\kappa < \infty$ fixed but letting the number of monomers $N \rightarrow \infty$, then

$$D(\kappa) := \lim_{N \rightarrow \infty} \frac{\mathcal{D}}{N} = \lambda^2 \frac{1 + \sigma}{1 - \sigma}, \quad (2.18c)$$

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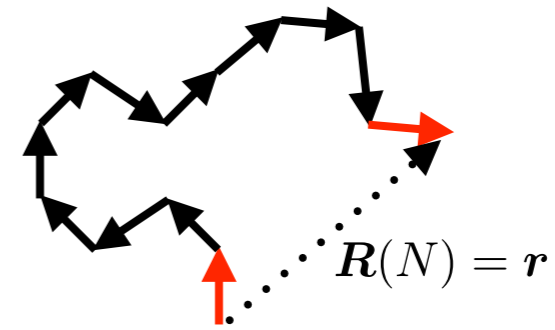
This means that, for finite κ , the end-to-end distance increases with $N^{1/2}$ corresponding to normal diffusion. For floppy polymers with $\kappa \rightarrow 0$, one finds that $D \rightarrow \lambda^2$, whereas for large κ

$$\lim_{\kappa \rightarrow \infty} \frac{D}{\kappa} = 2\lambda^2. \quad (2.19)$$

That is, for long stiff polymers with $\kappa \gg 1$, we have

$$D \simeq 2\lambda^2 \kappa = 2\lambda L_P. \quad (2.20)$$

Excursion PDF & thermodynamics



$$p_N(\mathbf{r}) = \mathbb{E}[\delta(\mathbf{r} - \mathbf{R}(N))]$$

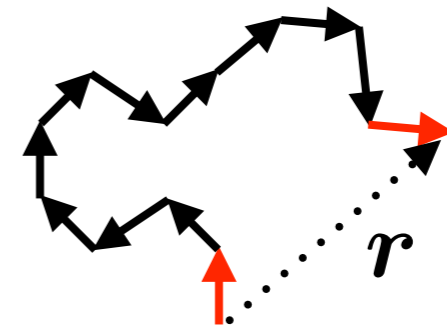
Unfortunately, it is not possible to compute the excursion PDF (2.7c) exactly for the vMF model¹. However, the central limit theorem combined with (2.18c) implies that, for large N , the excursion PDF will approach a Gaussian

$$p(\mathbf{r}) \simeq \left(\frac{3}{2\pi DN} \right)^{3/2} e^{-3\mathbf{r}^2/(2DN)}. \quad (2.21)$$

For the remainder of this section, we will assume that the end-points of the polymer are fixed at $\mathbf{0}$ and \mathbf{r} . To make the connection with thermodynamics, we may consider \mathbf{r} as a *macroscopic* state-variable, that can be realized by a number of different polymer configurations referred to as *microstates*. If no other constraints are known, it is plausible that each microstate is equally likely and, for large N , the number of microstates realizing a specific the macrostate \mathbf{r} is $\lambda^3 p(\mathbf{r})$, assuming the spatial resolution is of the order of the segment length λ . The corresponding microcanonical entropy is given by

$$S \simeq k_B \ln[\lambda^3 p(\mathbf{r})] = S_0 - k_B \frac{3\mathbf{r}^2}{2DN}. \quad (2.22)$$

Excursion PDF & thermodynamics



$$S \simeq k_B \ln[\lambda^3 p(\mathbf{r})] = S_0 - k_B \frac{3r^2}{2DN}$$

To obtain a prediction for the mean force \mathbf{f} required to stretch the polymer by a small amount $d\mathbf{r}$, we can exploit the general thermodynamic relation

$$dE = \delta W + \delta Q, \quad (2.23a)$$

where work and heat increments are defined as usual by

$$\delta W = -\mathbf{f} \cdot d\mathbf{r}, \quad \delta Q = TdS, \quad (2.23b)$$

with T denoting temperature. If one neglect self-avoidance interactions, which are present in real polymers, the energy remains constant during a change of conformation, $dE = 0$. Hence,

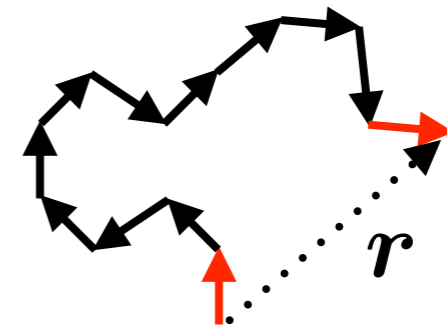
$$dS = \frac{\mathbf{f}}{T} \cdot d\mathbf{r} \quad (2.24)$$

and the stretch force components are obtained as

$$f_i = T \left(\frac{\partial S}{\partial r_i} \right) = -\frac{3k_B T}{DN} r_i. \quad (2.25)$$

$-\mathbf{f}$ is the force needed to stretch a polymer in a solvent bath of temperature T

Excursion PDF & thermodynamics



$$S \simeq k_B \ln[\lambda^3 p(\mathbf{r})] = S_0 - k_B \frac{3\mathbf{r}^2}{2DN}$$

Furthermore, it is also instructive to compute the corresponding free-energy

$$F := E - TS = E - TS_0 + k_B T \frac{3\mathbf{r}^2}{2DN}. \quad (2.26)$$

This is essentially a thermodynamic version of Hooke's law

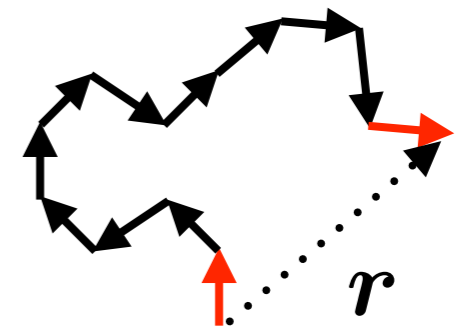
$$F = F_0 + \frac{K}{2} \mathbf{r}^2, \quad K = \frac{3k_B T}{DN}. \quad (2.27)$$

For long stiff polymers we have $DN \simeq 2\lambda N L_P = 2LL_P$, we find for the spring-constant

$$K = \frac{3k_B T}{2LL_P}. \quad (2.28)$$

This means, for example, that the persistence length L_p can be inferred from force measurements if temperature T and polymer length L are known.

Self-avoidance (Flory's scaling argument)

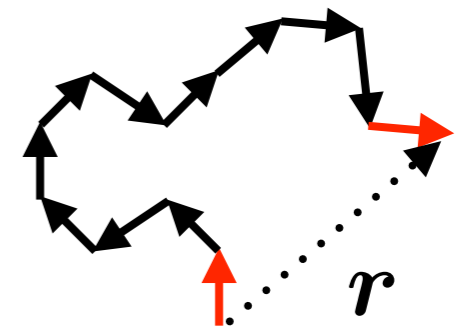


$$F = F_0 + \frac{K}{2} \mathbf{r}^2, \quad K = \frac{3k_B T}{DN}$$

- IDEA: include additional free energy term to account for self repulsion
- ASSUMPTIONS:
 - (i) $N \gg 1$ monomers of volume v_d with fixed end-to-end distance \mathbf{r}
 - (ii) for a fixed $|\mathbf{r}|$, the N monomers may (very roughly) explore a volume of $|\mathbf{r}|^d$,
 - (iii) overlap probability given by volume filling fraction $\phi = v_d N / |\mathbf{r}|^d$

$$F_e \simeq Nk_B T \phi = Nk_B T \frac{v_d N}{|\mathbf{r}|^d} \quad \Rightarrow \quad F = F_0 + Nk_B T \left(\frac{v_d N}{|\mathbf{r}|^d} + \frac{|\mathbf{r}|^2 d}{2D_d N^2} \right)$$

Self-avoidance (Flory's scaling argument)



$$F = F_0 + Nk_B T \left(\frac{v_d N}{|\mathbf{r}|^d} + \frac{|\mathbf{r}|^2 d}{2D_d N^2} \right). \quad (2.30)$$

To obtain the equilibrium distance r_* , we must minimize this expression with respect to $r = |\mathbf{r}|$, which gives

$$0 = \frac{dF}{d|\mathbf{r}|} = -d \frac{v_d N}{r_*^{d+1}} + \frac{d}{D_d N^2} r_* \quad (2.31)$$

and therefore

$$r_* = (D_d v_d)^{1/d+2} N^{3/(d+2)}. \quad (2.32)$$

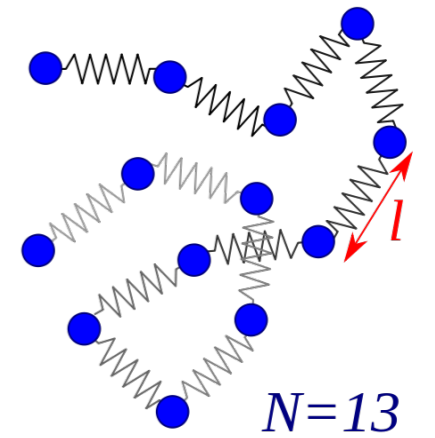
Thus, explicitly

$$d = 1 : \quad r_* \propto N \quad (2.33a)$$

$$d = 2 : \quad r_* \propto N^{3/4}, \quad (2.33b)$$

$$d = 3 : \quad r_* \propto N^{3/5}. \quad (2.33c)$$

The result is trivial for $d = 1$, seems to be exact for $d = 2$ when compared to simulations, and is very close to best numerical results $N^{0.589\dots}$ for $d = 3$.



2.2 Bead-spring model

single bead is governed by the over-damped Langevin equation

$$d\mathbf{X}_\alpha(t) = -\nabla_{\mathbf{x}_\alpha} U(\{\mathbf{X}_\alpha\}) dt + \sqrt{2D} * d\mathbf{B}_\alpha(t), \quad (2.34)$$

where D is the thermal diffusion constant of a bead. The potential U contains contributions from elastic nearest neighbor interactions U_e , from bending U_b and, to implement self-avoidance, steric short-range repulsion U_s :

$$U = U_e + U_b + U_s \quad (2.35)$$

Defining $(N - 1)$ chain link vectors \mathbf{R}_α and their orientations $\boldsymbol{\mu}_\alpha$ by

$$\mathbf{R}_\alpha = \mathbf{X}_{\alpha+1} - \mathbf{X}_\alpha, \quad \boldsymbol{\mu}_\alpha = \frac{\mathbf{R}_\alpha}{\|\mathbf{R}_\alpha\|} \quad (2.36)$$

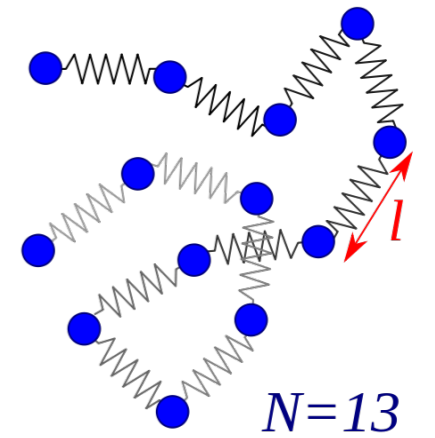
the potentials can be written as sums over 2-body and 3-body interactions

$$U_e = \sum_{\alpha=1}^{N-1} u(\|\mathbf{R}_\alpha\|), \quad U_b = \sum_{\alpha=1}^{N-2} b(\boldsymbol{\mu}_\alpha \cdot \boldsymbol{\mu}_{\alpha+1}), \quad U_s = \sum_{\alpha=1}^N \sum_{\beta=1, \beta \neq \alpha}^N s(\|\mathbf{X}_\alpha - \mathbf{X}_\beta\|).$$

Specifically, the elastic spring potential $u(r)$ and the steric repulsion potential $s(r)$ encode 2-body interactions, whereas the bending potential $b(q)$ involves 3-body interactions.²

Plausible choices are

$$u(r) = \frac{K}{2}(r - \lambda)^2, \quad b(q) = \frac{B}{2}(q - 1)^2, \quad s(r) = \frac{S e^{-r/\sigma}}{r^\nu} \quad (2.38)$$



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Needs to be solved numerically but **stationary distribution known**

$$p_N(\{\mathbf{x}_\alpha\}) = \frac{1}{Z_N} \exp\left[-\frac{U(\{\mathbf{X}_\alpha\})}{D}\right], \quad (2.39)$$

where

$$Z_N = \int \left(\prod_{\alpha=1}^N d^3x_\alpha \right) \exp\left[-\frac{U(\{\mathbf{x}_\alpha\})}{D}\right]. \quad (2.40)$$