A quantitative description of the invasion of bacteriophage T4

R. D. James
IMA and Aerospace Engineering and Mechanics
University of Minnesota

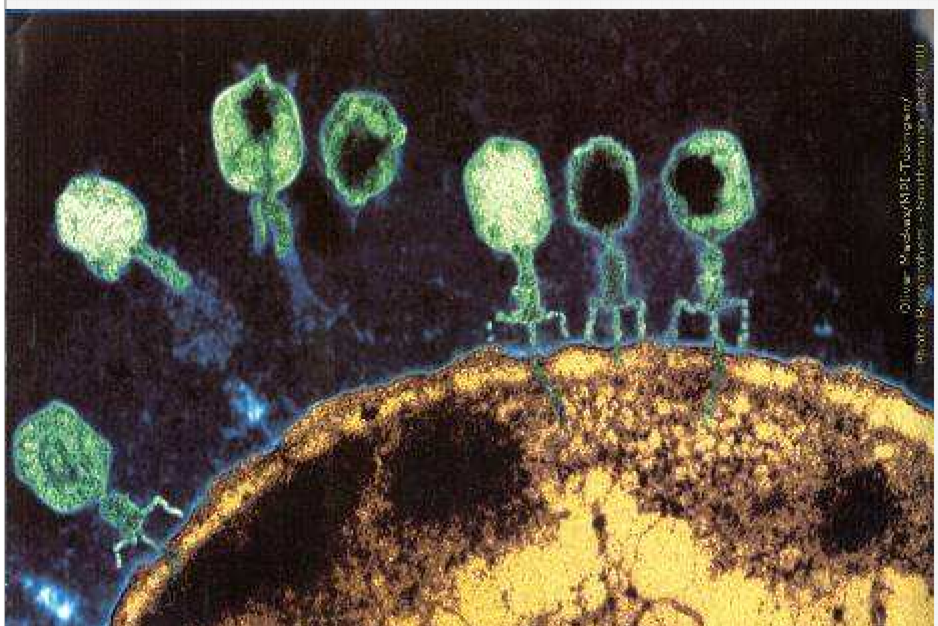
Joint work with Wayne Falk
Microbiology and Oral Science, University of Minnesota

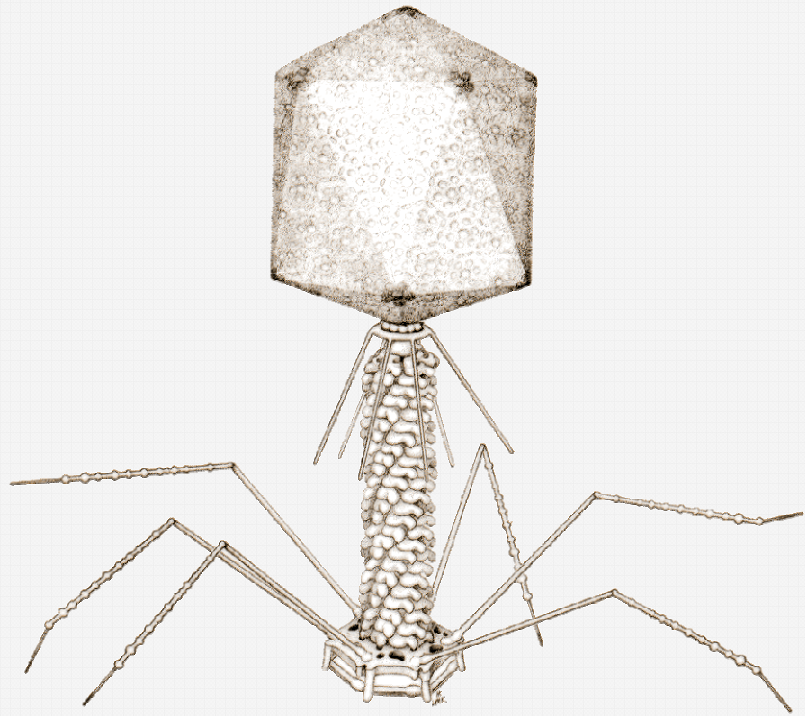
Thanks: John Maddocks, Rob Phillips

9 September, 2005

Bacteriophage T4: a virus that attacks bacteria

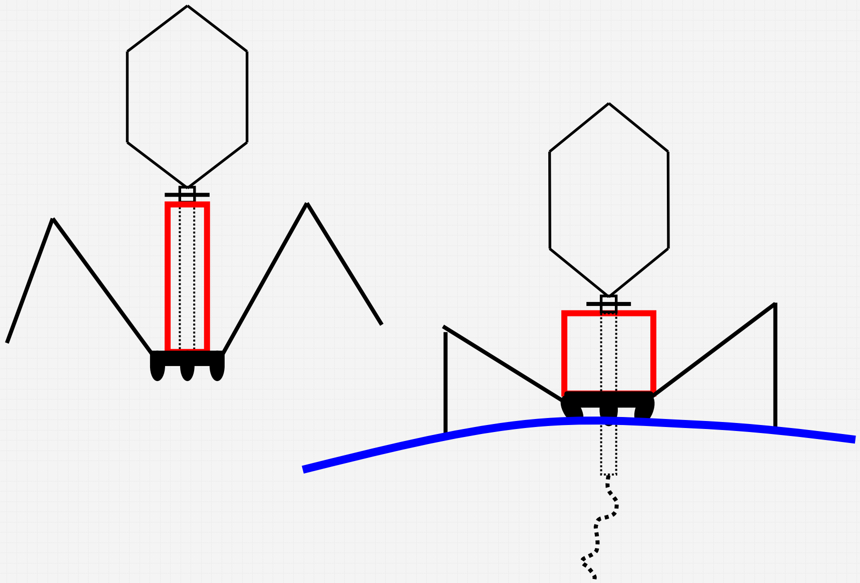
Bacteriophage T-4 attacking
a bacterium: phage at the right
is injecting its DNA

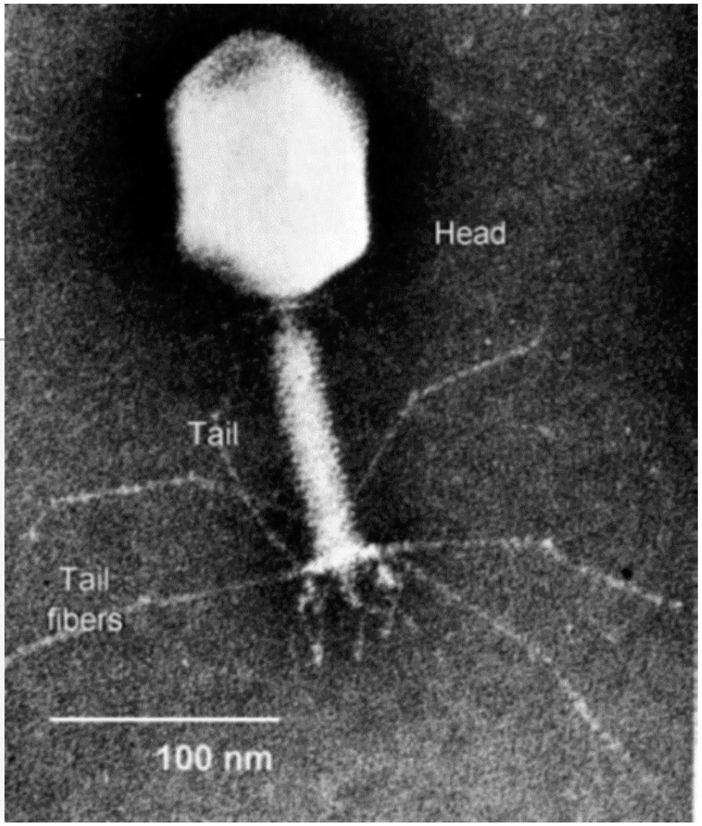


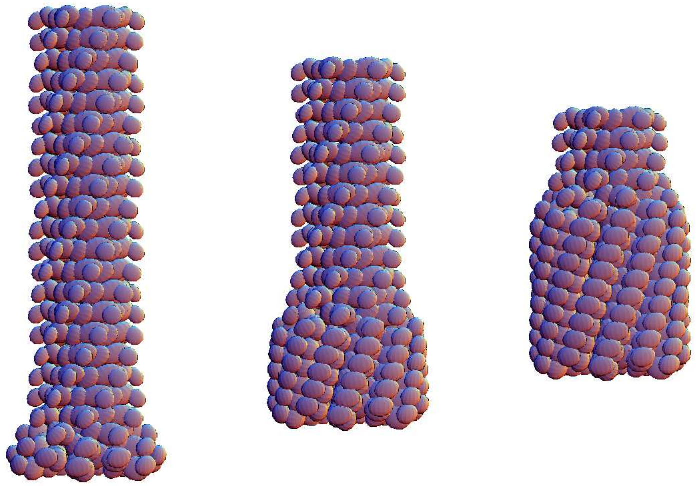


Wakefield, Julie (2000) The return of the phage. Smithsonian 31:42-6

Mechanism of infection







This talk mainly concerns the tail sheath

A 100nm bioactuator

Many interesting questions for quantitative analysis

- How much force is generated?
- Where does the energy (force x distance) come from?
- How does this energy compare with similar martensitic phase transformations in materials?
- What kind of elasticity theory is appropriate for a sheet of protein molecules?
- …that transforms?
- How is tail sheath made in Nature?
- How could one make tail sheath artificially?

Elasticity theory of protein lattices

Falk, James

- First principles approach: protein sequence known but folded protein structure not known, interactions with solution important, time scale of transformation could be long.
- Even if one could do a full, chemically accurate MD simulation for a sufficiently long time, would it answer any of the questions on the previous slide?

Our approach: focus at protein level. Assume each protein molecule is characterized by a position and orientation and build a free energy.

Definitions of position and orientation

Usual method (e.g., DeGennes, Chapt 2): moments of the mass distribution, e.g., 4th moment, 6th moment

Alternative approach:

$$\{\mathbf{q}, \ldots, \mathbf{q}_\nu\}$$

Positions of atoms in the molecule

$$\mathbf{y} = \frac{\sum_{i=1}^{\nu} m_i \, \mathbf{q}_i}{\sum_{i=1}^{\nu} m_i}$$

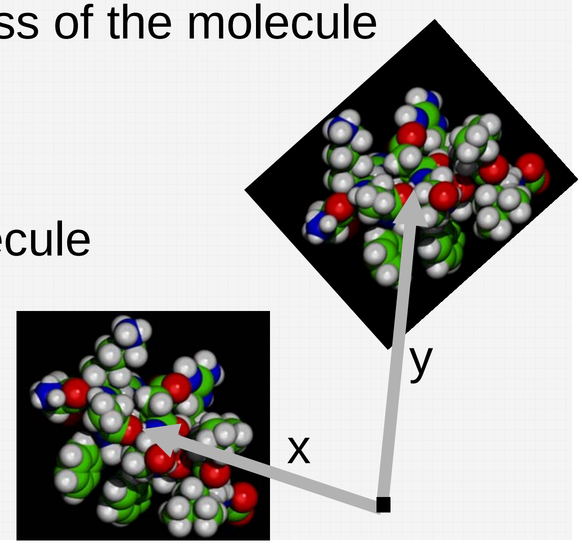
Position = center of mass of the molecule

$$\{\mathbf{x}, \ldots, \mathbf{x}_\nu\}$$

Positions of corresponding atoms in the reference molecule

$$\mathbf{x} = \frac{\sum_{i=1}^{\nu} m_i \, \mathbf{x}_i}{\sum_{i=1}^{\nu} m_i}$$

Center of mass of the reference molecule



Orientation

$$\mathbf{F} = \frac{\Sigma_{i=1}^{\nu} m_i \left(\mathbf{q}_i - \mathbf{y}\right) \otimes \left(\mathbf{x}_i - \mathbf{x}\right)}{r^2 \; \Sigma_{i=1}^{\nu} m_i} = \mathbf{R}\mathbf{U}$$

polar decomposition

Def: orientation

Properties:

1) Variational characterization

$$\min_{\mathbf{c}\,,\mathbf{Q}\in SO(3)} \int \left| \mathbf{q}(\mathbf{z}) - \left[\mathbf{Q}(\mathbf{z}-\mathbf{x}) + \mathbf{c}\right)\right] \right|^2 dm(\mathbf{z})$$

$$\Longrightarrow \quad \mathbf{Q} = \mathbf{R} \quad \text{and} \quad \mathbf{c} = \mathbf{y}$$

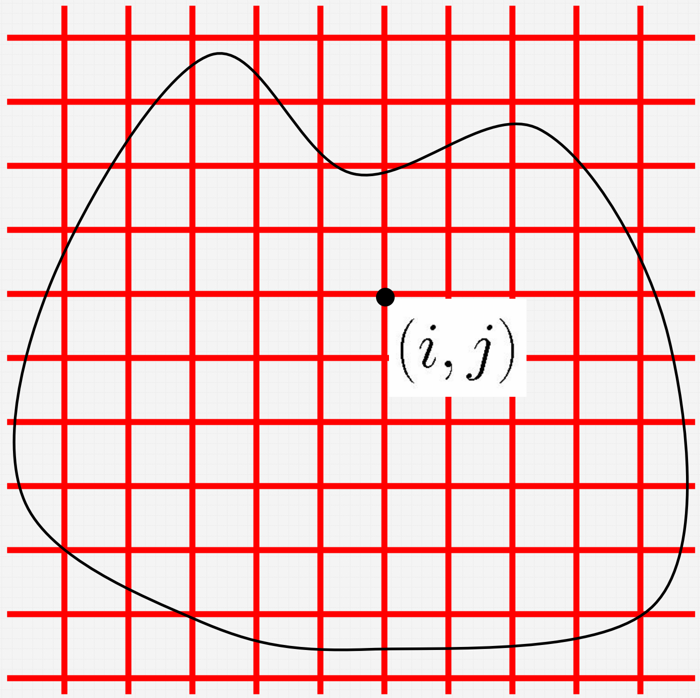
2) Constrained MD simulation

$$\mathbf{R} = \mathbf{F}\mathbf{U}^{-1} = \mathbf{F}(\sqrt{\mathbf{F}^T\mathbf{F}})^{-1}$$

$$\mathrm{Skew}\left(\mathbf{R}\left(\Sigma_{i=1}^{\nu} m_i \left(\mathbf{x}_i - \mathbf{x}\right) \otimes \left(\mathbf{q}_i - \mathbf{y}\right)\right)\right) = 0$$

(linear constraint)

Protein lattice



$$(\mathbf{y}_{i,j}, \mathbf{R}_{i,j})$$

$$(i,j) \in \Omega$$

Free energy

1) Chains:

$$\Psi(\mathbf{y}_1, \mathbf{R}_1, \ldots, \mathbf{y}_N, \mathbf{R}_N) = \sum_{i=2}^{N-2} \psi(\mathbf{y}_i, \mathbf{R}_i, \mathbf{y}_{i+1}, \mathbf{R}_{i+1}) + \text{free energy of boundary molecules}$$

2) Sheets: two bonding directions (i,j)-(i+1,j) and (i,j)-(i,j+1)

$$\Psi(\mathbf{y}_{1,1}, \mathbf{R}_{1,1}, \ldots, \mathbf{y}_{N,M}, \mathbf{R}_{N,M}) = \sum_{(i,j)\in\mathbb{Z}^2\cap\Omega\setminus\mathcal{B}} \psi_1(\mathbf{y}_{i,j}, \mathbf{R}_{i,j}, \mathbf{y}_{i+1,j}, \mathbf{R}_{i+1,j}) + \psi_2(\mathbf{y}_{i,j}, \mathbf{R}_{i,j}, \mathbf{y}_{i,j+1}, \mathbf{R}_{i,j+1}) + \text{free energy of boundary molecules}$$

Frame-indifference

$$\psi(\mathbf{y}_1, \mathbf{R}_1, \mathbf{y}_2, \mathbf{R}_2) = \psi(\mathbf{R}\mathbf{y}_1 + \mathbf{c}, \mathbf{R}\mathbf{R}_1, \mathbf{R}\mathbf{y}_2 + \mathbf{c}, \mathbf{R}\mathbf{R}_2)$$

$$\Updownarrow$$

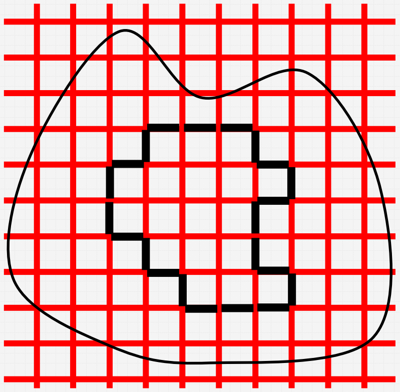
$$\psi(\mathbf{y}_1, \mathbf{R}_1, \mathbf{y}_2, \mathbf{R}_2) = \psi(0, \mathbf{I}, \mathbf{R}_1^T(\mathbf{y}_2 - \mathbf{y}_1), \mathbf{R}_1^T\mathbf{R}_2) = \varphi(\mathbf{t}, \mathbf{Q})$$

where $\mathbf{Q} = \mathbf{R}_1^T\mathbf{R}_2, \quad \mathbf{t} = \mathbf{R}_1^T(\mathbf{y}_1 - \mathbf{y}_2)$ "strain variables"

relative orientation relative position

Compatibility

Compatibility concerns the extent to which one can freely assign "strain variables".
Assume Ω is discretely simply connected.



Assume that:

$$(\mathbf{t}_{i,j}, \mathbf{Q}_{i,j}),\ (i,j) \in \Omega^r \quad \text{and} \quad (\hat{\mathbf{t}}_{i,j}, \hat{\mathbf{Q}}_{i,j}),\ (i,j) \in \Omega^u$$

Does there exist $\mathbf{y}_{i,j}, \mathbf{R}_{i,j},\ (i,j) \in \Omega$ such that

$$\begin{aligned}
\mathbf{t}_{i,j} &= \mathbf{R}_{i,j}^T(\mathbf{y}_{i+1,j} - \mathbf{y}_{i,j})\,, \\
\mathbf{Q}_{i,j} &= \mathbf{R}_{i,j}^T\mathbf{R}_{i+1,j}\,, && (i,j) \in \Omega^r, \\
\hat{\mathbf{t}}_{i,j} &= \mathbf{R}_{i,j}^T(\mathbf{y}_{i,j+1} - \mathbf{y}_{i,j})\,, \\
\hat{\mathbf{Q}}_{i,j} &= \mathbf{R}_{i,j}^T\mathbf{R}_{i,j+1}\,, && (i,j) \in \Omega^u
\end{aligned}$$

?

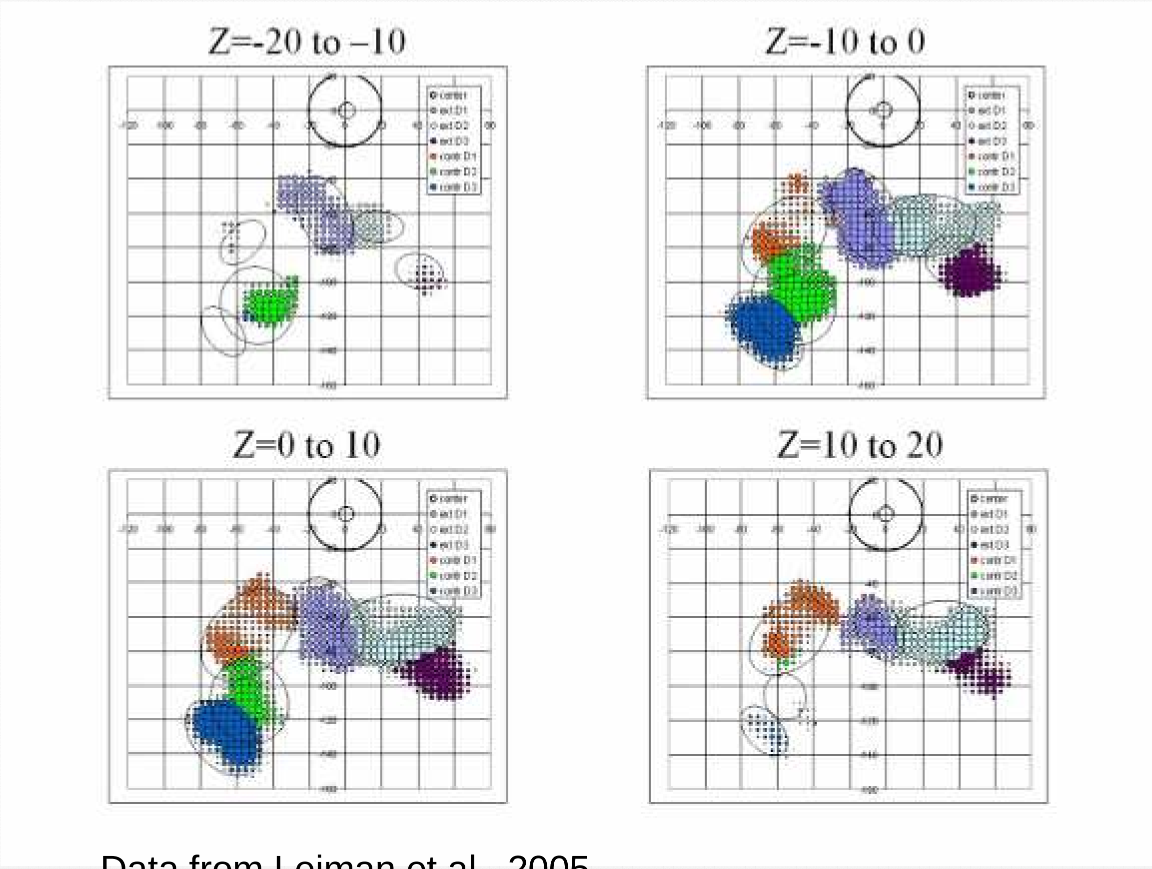
Necessary and sufficient conditions for compatibility

$$
\begin{aligned}
\hat{\mathbf{Q}}_{i,j}\mathbf{Q}_{i,j+1}\hat{\mathbf{Q}}^T_{i+1,j}\mathbf{Q}^T_{i,j} &= \mathbf{I},\\
\hat{\mathbf{t}}_{i,j} + \hat{\mathbf{Q}}_{i,j}\mathbf{t}_{i,j+1} - \mathbf{Q}_{i,j}\hat{\mathbf{t}}_{i+1,j} - \mathbf{t}_{i,j} &= 0
\end{aligned}
$$

(More bonding directions? These conditions above already determine all the positions and orientations up to overall rigid motion, which determines all other (t*,Q*) for all other bonding directions. One can write formulas for the (t*,Q*) corresponding to other bonding directions in terms of (t,Q, $\hat{t}$, $\hat{Q}$).)

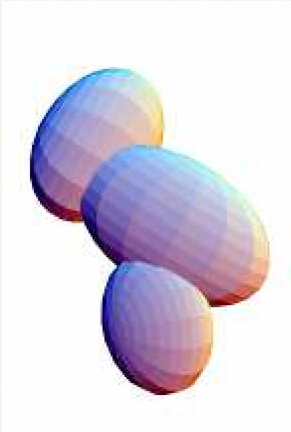
Structure of T4 sheath

1) Approximation of molecules using electron density maps



Data from Leiman et al., 2005

Gives orientation and position of one molecule in extended and contracted sheath

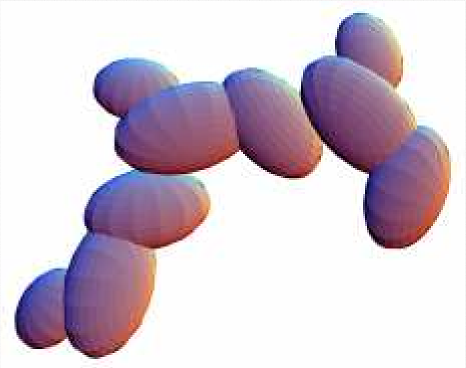


one molecule of extended sheath

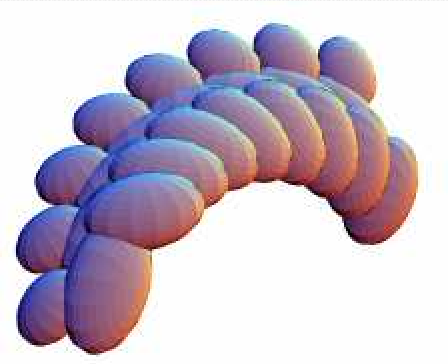
Structure of T4 sheath

2) Helices I: the 8/3 rule

3 consecutive molecules on the lowest annulus



8 consecutive molecules on the main helix



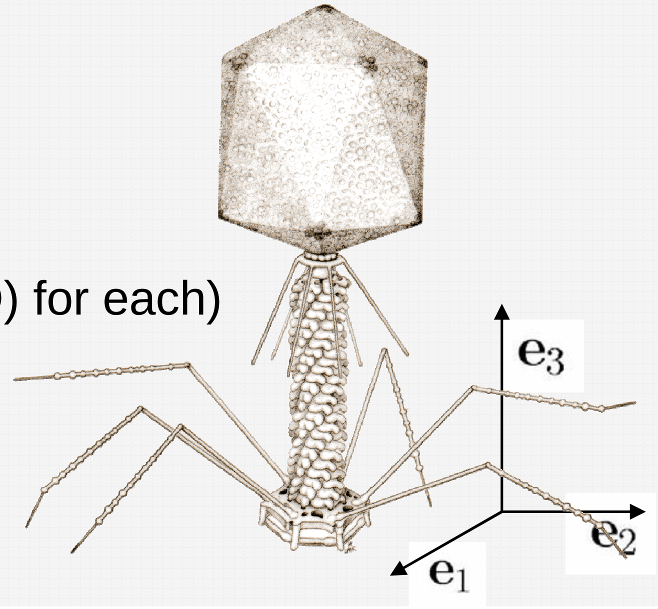
For contracted sheath there is a similar 12/1 rule

$$\mathbf{y}_{1,8} \cdot \mathbf{e}_1 = \mathbf{y}_{3,1} \cdot \mathbf{e}_1, \quad \mathbf{y}_{1,8} \cdot \mathbf{e}_2 = \mathbf{y}_{3,1} \cdot \mathbf{e}_2$$

3) Helices II: formulas for the helices (identify (t,Q) for each)

Let

$$\mathbf{Q}_\theta = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$



Structure of T4 sheath

$$\begin{aligned}
\mathbf{R}_{i,j} &= \mathbf{Q}_{\pi/3}^{i-1}\mathbf{Q}_{\gamma}^{j-1}\mathbf{R}_{1,1}, \\
\mathbf{y}_{i,j} &= \mathbf{y}_1 + \sum_{k=0}^{i-2}\mathbf{Q}_{\pi/3}^{k}\mathbf{t}_0 + \mathbf{Q}_{\pi/3}^{i-1}\sum_{k=0}^{j-2}\mathbf{Q}_{\gamma}^{k}\mathbf{t}, \\
& \quad i = 1,\ldots,6, \quad j = 1,\ldots,23,
\end{aligned}$$

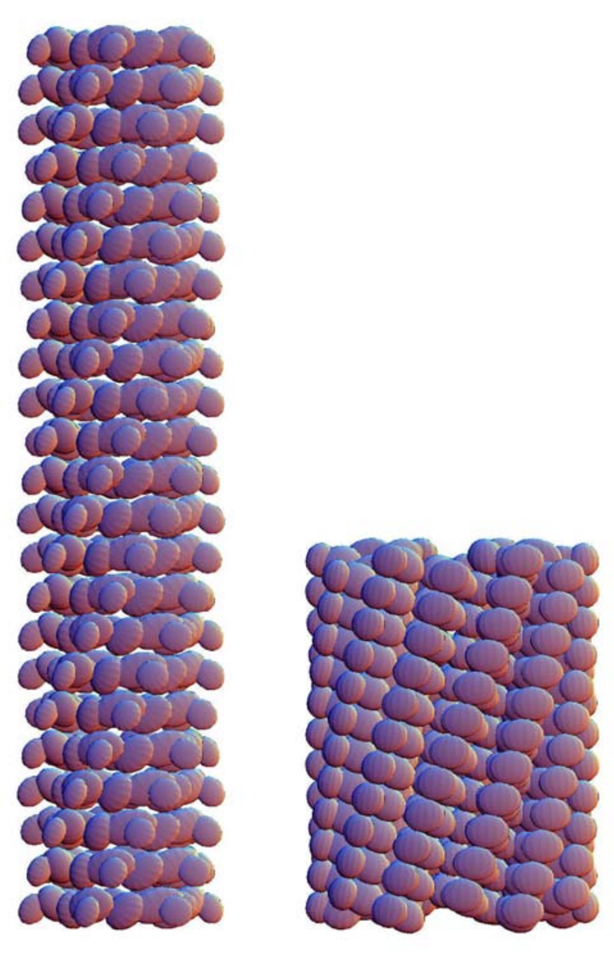
where,

$$\mathbf{y}_1 = \rho\,(1/2, \sqrt{3}/2, 0)$$

$$\mathbf{t}_0 = (-\rho, 0, 0)$$

$$\mathbf{t} = \lambda\mathbf{e}_3 + (\mathbf{Q}_\gamma - \mathbf{I})\mathbf{y}_1$$

Parameters: $\gamma, \quad \rho, \quad \lambda, \quad \mathbf{R}_{1,1}$



Values of the parameters

Extended sheath: $\gamma = 2\pi/21, \quad \rho = 73.75\ \text{Å}, \quad \lambda = 40.6\ \text{Å}, \quad \mathbf{R}_{1,1} = \mathbf{I}$

Contracted sheath: $\gamma = 2\pi/11, \quad \rho = 116.1\ \text{Å}, \quad \lambda = 16.4\ \text{Å}$

$$\mathbf{R}_{1,1} = \begin{pmatrix} 0.426 & 0.4388 & -0.791 \\ -0.4378 & 0.8653 & 0.244 \\ 0.7916 & 0.242 & 0.561 \end{pmatrix}$$

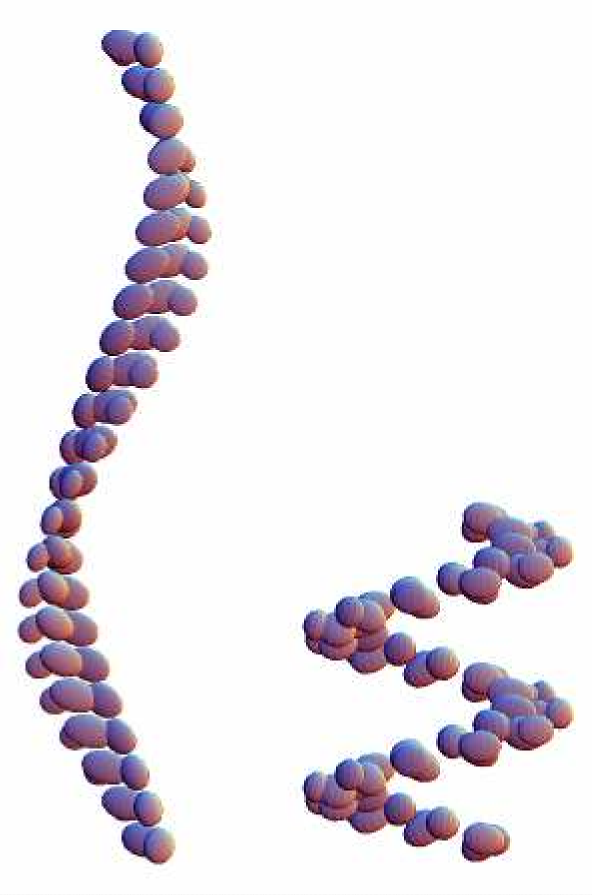
Even for homogeneous states there are lots of parameters. Is there a way to further simplify the free energy, accounting for special stiffnesses of T4 sheath?

$$\gamma, \quad \rho, \quad \lambda, \quad \mathbf{R}_{1,1}$$

Constrained theory I

Falk, James

The main helix:



Compute, for the main helix:

$$|\mathbf{t}|^2 = |\mathbf{R}^T_{i,j}(\mathbf{y}_{i,j+1} - \mathbf{y}_{i,j})|^2 = \lambda^2 + 2\rho^2(1 - \cos\gamma).$$

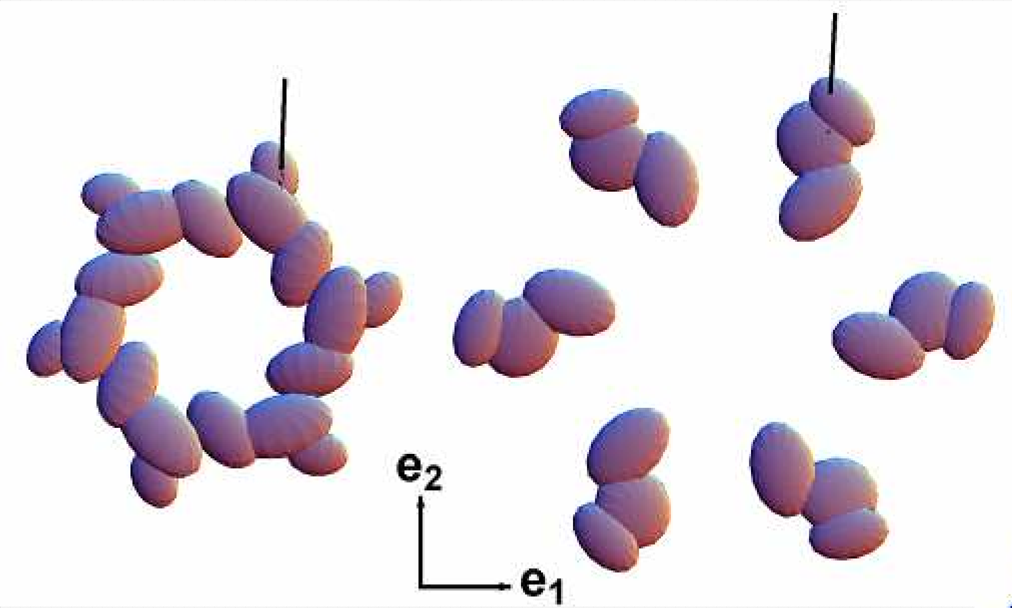
Observe:

$$\lambda^2 + \gamma^2\rho^2_{\text{eff}} = \begin{cases} 2170 \text{ Å}^2 & \text{for extended sheath,} \\ 2170 \text{ Å}^2 & \text{for contracted sheath.} \end{cases}$$

Assume above is true for all states.

Constrained theory II

Now look at the rotation of molecules:



Axis of rotation very near:

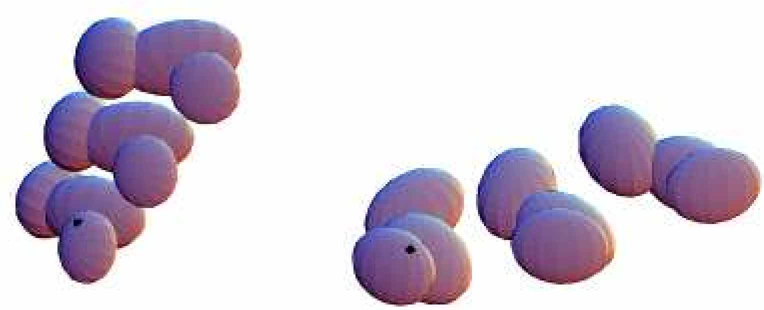
$$(0, \sqrt{3}/2, 1/2)$$

Assume:

$$\mathbf{R}_{1,1}(\theta) = \begin{pmatrix} \cos\theta & \frac{1}{2}\sin\theta & -\frac{\sqrt{3}}{2}\sin\theta \\ -\frac{1}{2}\sin\theta & \frac{3}{4}+\frac{1}{4}\cos\theta & \frac{\sqrt{3}}{4}-\frac{\sqrt{3}}{4}\cos\theta \\ \frac{\sqrt{3}}{2}\sin\theta & \frac{\sqrt{3}}{4}-\frac{\sqrt{3}}{4}\cos\theta & \frac{1}{4}+\frac{3}{4}\cos\theta \end{pmatrix}.$$

Note:

$$\mathbf{e}_1 \cdot \mathbf{R}_{1,1}^T(\theta)(\mathbf{y}_{1,2} - \mathbf{y}_{1,1}) = \begin{cases} -21.2\ \text{Å} & \text{for extended sheath,} \\ -21.2\ \text{Å} & \text{for contracted sheath.} \end{cases}$$

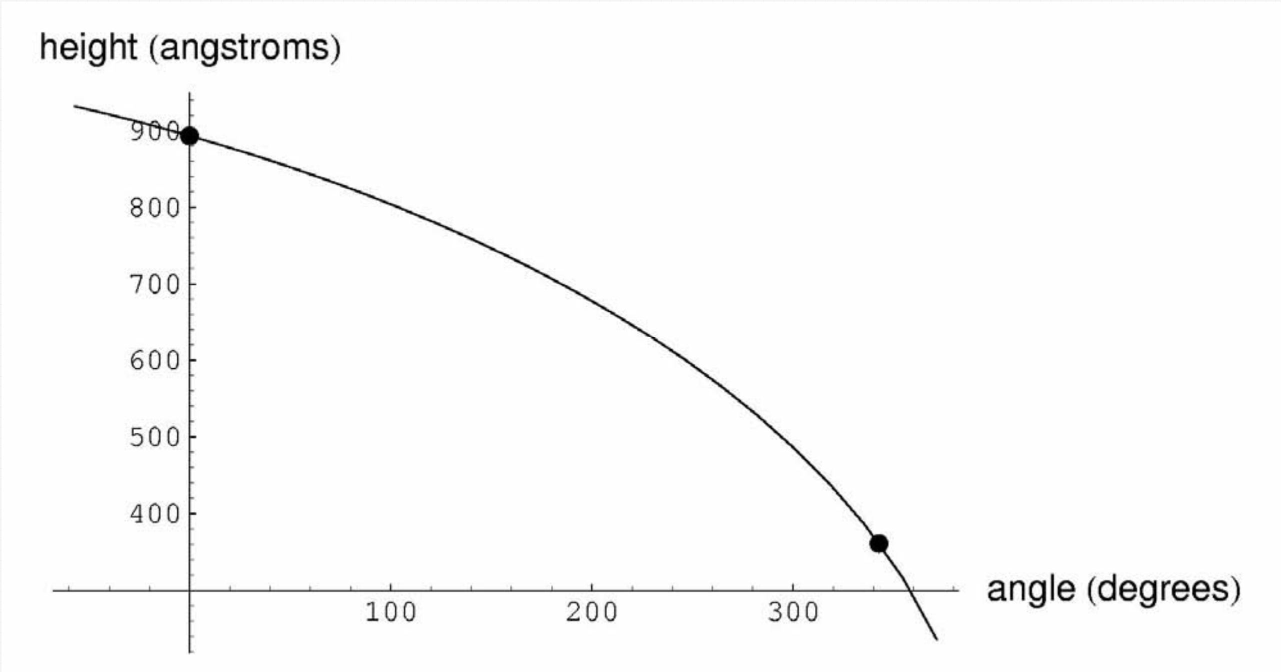


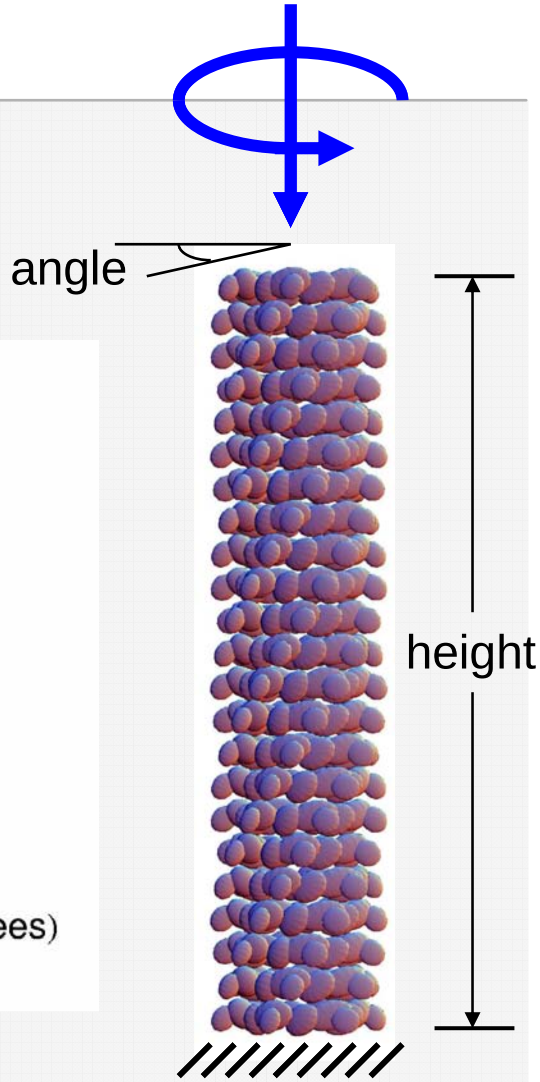
Assume: $$2\rho\cos\theta\left(1+\sqrt{3}\sin\gamma - \cos\gamma\right) + \sin\theta\left(\rho\sin\gamma + \rho\sqrt{3}\cos\gamma - \sqrt{3}(2\lambda+\rho)\right) = 84.8\ \text{Å}$$

Summary: the main helix dominates

Consequence of constraint I: an unusual Poynting effect

$$\lambda^2 + \gamma^2 \rho_{\text{eff}}^2 = 2170 \ \text{Å}^2$$





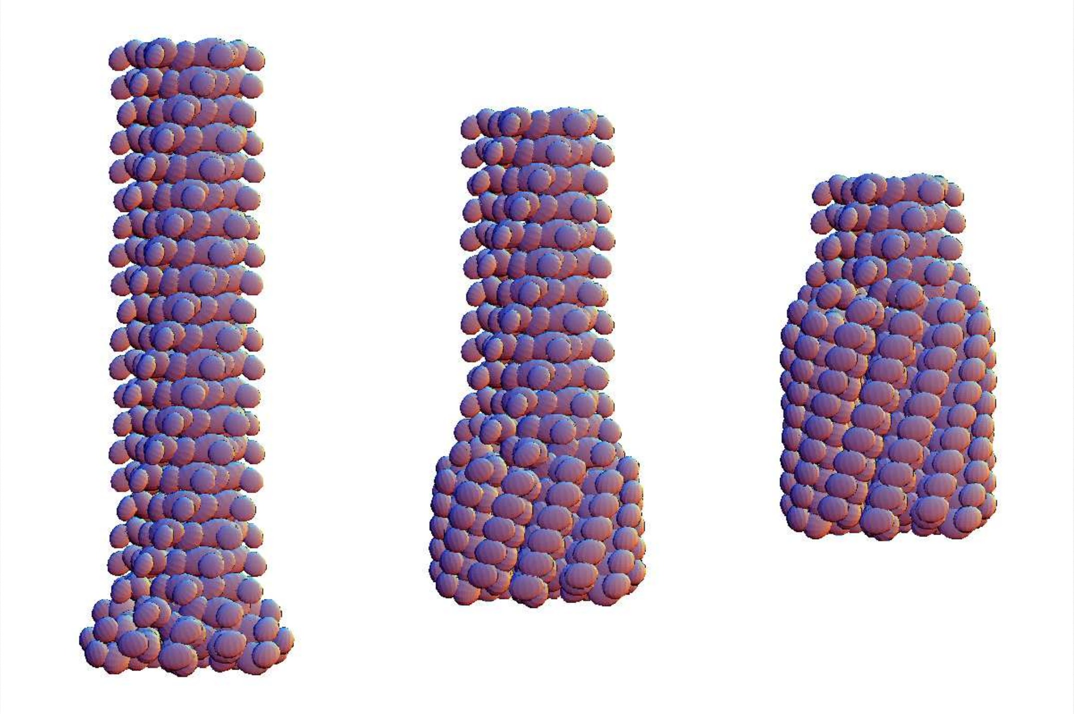
Nonuniform states

$$\begin{aligned}\mathbf{R}_{i,j} &= \mathbf{Q}_{\pi/3}^{i-1}\mathbf{Q}_{\gamma}^{j-1}\mathbf{R}_{1,1},\\ \mathbf{y}_{i,j} &= \mathbf{y}_1 + \sum_{k=0}^{i-2}\mathbf{Q}_{\pi/3}^{k}\mathbf{t}_0 + \mathbf{Q}_{\pi/3}^{i-1}\sum_{k=0}^{j-2}\mathbf{Q}_{\gamma}^{k}\mathbf{t}, \quad (\star)\\ & i=1,\dots,6, \quad j=1,\dots,23.\end{aligned}$$

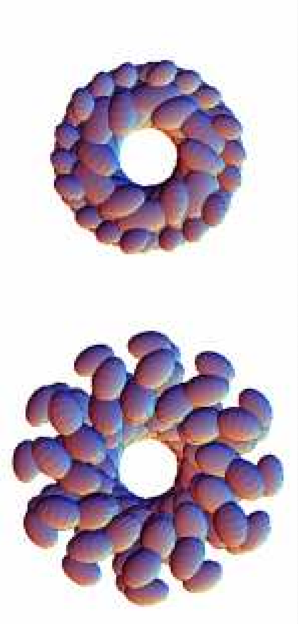
$$(\mathbf{y}_{i,j}, \mathbf{R}_{i,j}) \text{ is given by } (\star) \text{ with } \rho=\rho_j,\ \gamma=\gamma_j,\ \lambda=\lambda_j,\ \mathbf{R}_{1,1}=\mathbf{R}_j,$$
$$i=1,\dots,6,\ j=1,\dots,23.$$

(1D ansatz)

transition layer by simple linear interpolation

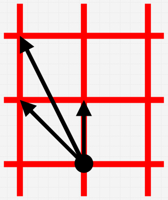


nucleation



Simplified free energy

T4 sheath has three important bonding directions



$$\Psi(\mathbf{y}_{1,1}, \mathbf{R}_{1,1}\ , \ldots ,\ \mathbf{y}_{6,23}, \mathbf{R}_{6,23})$$
$$= \sum_{i\in\{1,\ldots,6\},\ j\in\{1,\ldots,23\}} \psi_1(\mathbf{y}_{i,j}, \mathbf{R}_{i,j}, \mathbf{y}_{i,j+1}, \mathbf{R}_{i,j+1}) + \psi_2(\mathbf{y}_{i,j}, \mathbf{R}_{i,j}, \mathbf{y}_{i-1,j+1}, \mathbf{R}_{i-1,j+1})$$
$$+ \psi_3(\mathbf{y}_{i,j}, \mathbf{R}_{i,j}, \mathbf{y}_{i-1,j+2}, \mathbf{R}_{i-1,j+2})$$

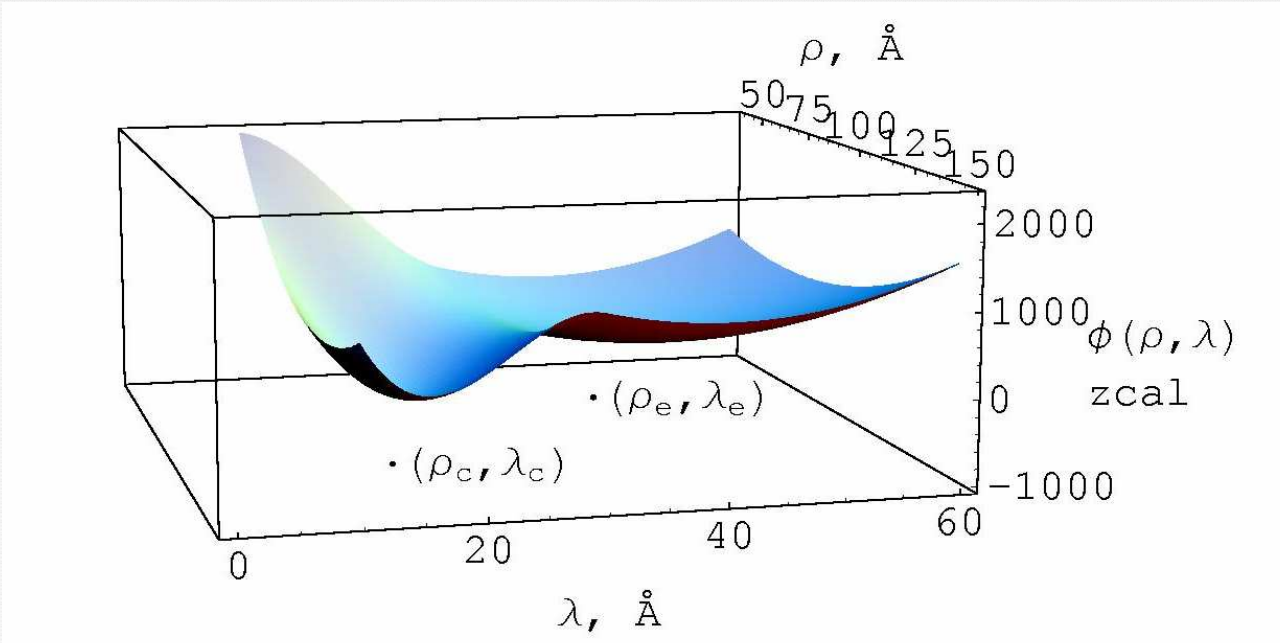
$$\Psi(\mathbf{y}_{1,1}, \mathbf{R}_{1,1}\ , \ldots ,\ \mathbf{y}_{6,23}, \mathbf{R}_{6,23}) = \sum_{j\in\{1,\ldots,23\}} \psi(\rho_j, \rho_{j+1}, \rho_{j+2}, \bar{\lambda}_j, \bar{\lambda}_{j+1})$$

$$\phi(\rho, \lambda) = \psi(\rho, \rho, \rho, \lambda, \lambda)$$

Simplified free energy, continued

Arisaka, Engle and Klump did calorimetry on T4 sheath, measuring the heat released on contraction. Thermodynamics + approximations:

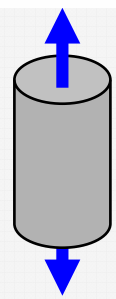
$$\phi(\rho_e, \lambda_e) - \phi(\rho_c, \lambda_c) = 60 \text{ zcal/annulus.}$$



Some linearized calculations

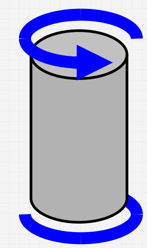
$$\phi_c(\rho,\lambda) = \phi_c^0 + \frac{1}{2}\left(A(\rho-\rho_c)^2 + 2B(\rho-\rho_c)(\lambda-\lambda_c) + C(\lambda-\lambda_c)^2\right) + \dots$$

$$\text{tensile modulus} = \frac{\lambda_c^2(AC-B^2)}{A}$$



$$\Psi(\mathbf{y}_{1,1},\mathbf{R}_{1,1},\dots,\mathbf{y}_{6,23},\mathbf{R}_{6,23}) - \mathbf{y}_{1,23}\cdot\mathbf{f}$$
$$= \Psi(\mathbf{y}_{1,1},\mathbf{R}_{1,1},\dots,\mathbf{y}_{6,23},\mathbf{R}_{6,23}) - 22\, f\, \lambda_{23}$$

$$\text{Poisson's ratio} = \frac{1-\frac{\rho}{\rho_c}}{\frac{\lambda}{\lambda_c}-1} = \frac{\lambda_c}{\rho_c}\frac{B}{A}$$

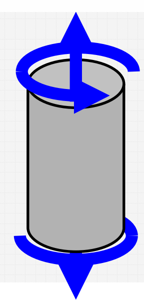


$$\text{torsional modulus} = \frac{\text{moment}}{\text{twist/length}} = \frac{\gamma_c^2\,\rho_{eff}^4(AC-B^2)}{A}$$

Rigidity:

$$f \to f + f_1, \quad M \to M + M_1$$

$$M_1 = -\frac{d\lambda}{d\gamma}\, f_1 = \frac{\rho_{eff}^2\tilde{\gamma}}{\tilde{\lambda}}\, f_1$$



Fully relaxed states

No boundary conditions, try to minimize energy by hand

$$\Psi(\mathbf{y}_{1,1}, \mathbf{R}_{1,1}, \ldots, \mathbf{y}_{N,M}, \mathbf{R}_{N,M}) = \sum_{(i,j)\in\mathbb{Z}^2\cap\Omega} \psi_1(\mathbf{y}_{i,j}, \mathbf{R}_{i,j}, \mathbf{y}_{i+1,j}, \mathbf{R}_{i+1,j}) + \psi_2(\mathbf{y}_{i,j}, \mathbf{R}_{i,j}, \mathbf{y}_{i,j+1}, \mathbf{R}_{i,j+1})$$

Try

$$\left.\begin{array}{l} \mathbf{t}_{i,j} = \mathbf{t}, \\ \mathbf{Q}_{i,j} = \mathbf{Q}, \\ \hat{\mathbf{t}}_{i,j} = \hat{\mathbf{t}}, \\ \hat{\mathbf{Q}}_{i,j} = \hat{\mathbf{Q}}, \end{array}\right\} \quad \text{where} \quad \left\{\begin{array}{ll} \tilde{\psi}_1(\mathbf{t}, \mathbf{Q}) \le \tilde{\psi}_1(\mathbf{a}, \mathbf{R}) & \text{for all} \quad (\mathbf{a}, \mathbf{R}), \\ \tilde{\psi}_2(\hat{\mathbf{t}}, \hat{\mathbf{Q}}) \le \tilde{\psi}_2(\hat{\mathbf{a}}, \hat{\mathbf{R}}) & \text{for all} \quad (\hat{\mathbf{a}}, \hat{\mathbf{R}}), \end{array}\right.$$

To be able to reconstruct the positions and orientations must satisfy compatibility:

$$\begin{aligned} \hat{\mathbf{Q}}\mathbf{Q}\hat{\mathbf{Q}}^T\mathbf{Q}^T &= \mathbf{I}, \\ \hat{\mathbf{t}} + \hat{\mathbf{Q}}\mathbf{t} - \mathbf{Q}\hat{\mathbf{t}} - \mathbf{t} &= 0. \end{aligned}$$

FRUSTRATION

Fully relaxed states

Assume the minimizers of the "integrand" do satisfy

$$\begin{aligned} \hat{\mathbf{Q}}\mathbf{Q}\hat{\mathbf{Q}}^T\mathbf{Q}^T &= \mathbf{I}, \\ \hat{\mathbf{t}} + \hat{\mathbf{Q}}\mathbf{t} - \mathbf{Q}\hat{\mathbf{t}} - \mathbf{t} &= 0. \end{aligned}$$

Solution:

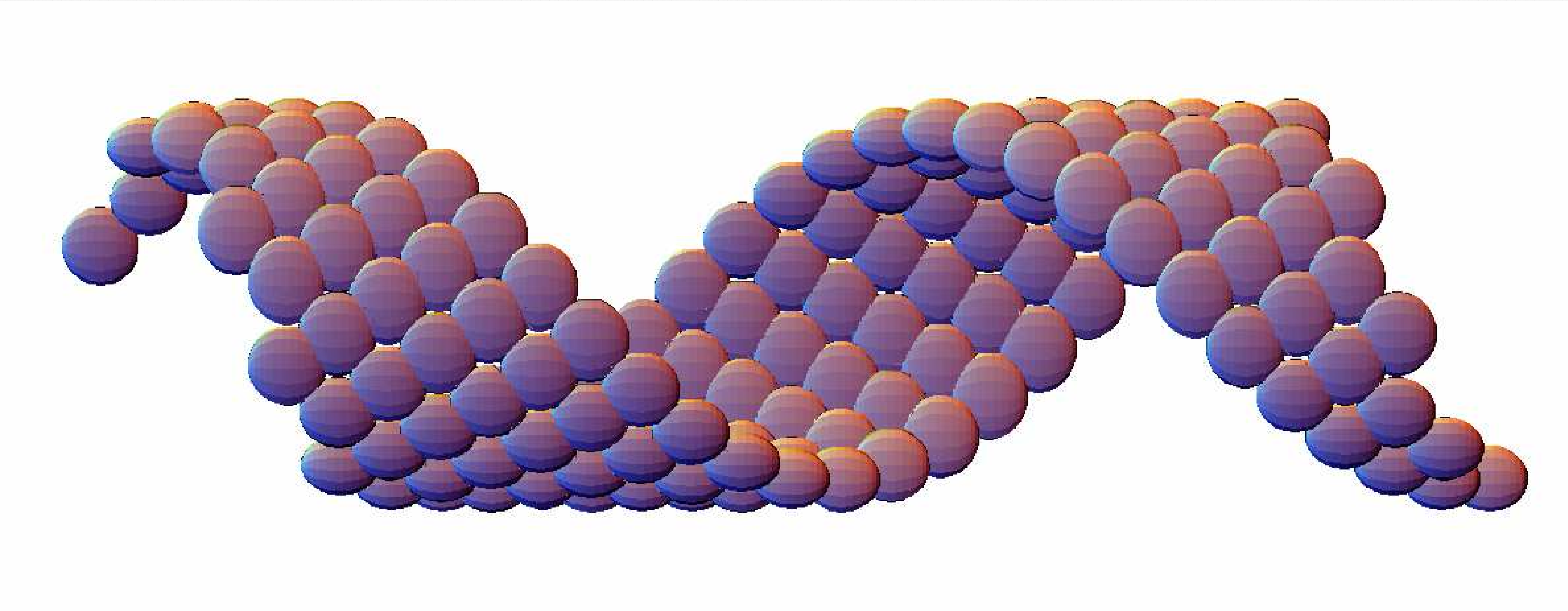
1. $\mathbf{Q}$ and $\hat{\mathbf{Q}}$ are coaxial, $\mathbf{Q}\mathbf{e} = \hat{\mathbf{Q}}\mathbf{e} = \mathbf{e}$, $|\mathbf{e}| = 1$, and
   (a) If $\mathbf{Q} \neq \mathbf{I}$ and $\hat{\mathbf{Q}} \neq \mathbf{I}$, then $\mathbf{t} = \mathbf{t}_1 + \tau\mathbf{e}$ and $\hat{\mathbf{t}} = \hat{\mathbf{t}}_1 + \tau\mathbf{e}$ for some τ with $\mathbf{t}_1 \cdot \mathbf{e} = \hat{\mathbf{t}}_1 \cdot \mathbf{e} = 0$, and $\hat{\mathbf{t}}_1 = (\mathbf{I} - \mathbf{Q})^{-1}(\mathbf{I} - \hat{\mathbf{Q}})\mathbf{t}_1$, the inverse taken on the plane perpendicular to $\mathbf{e}$.
   (b) If $\mathbf{Q} \neq \mathbf{I}$ and $\hat{\mathbf{Q}} = \mathbf{I}$, then $\mathbf{t}$ is arbitrary but $\hat{\mathbf{t}} = \tau\mathbf{e}$ for some τ.
   (c) If $\mathbf{Q} = \mathbf{I}$ and $\hat{\mathbf{Q}} \neq \mathbf{I}$, then $\hat{\mathbf{t}}$ is arbitrary but $\mathbf{t} = \tau\mathbf{e}$ for some τ.
   (d) If $\mathbf{Q} = \mathbf{I}$ and $\hat{\mathbf{Q}} = \mathbf{I}$, then $\hat{\mathbf{t}}$ and $\mathbf{t}$ are arbitrary.
2. (Degenerate case) $\mathbf{Q} = \mathbf{I} - 2\mathbf{e} \otimes \mathbf{e}$ and $\hat{\mathbf{Q}} = \mathbf{I} - 2\hat{\mathbf{e}} \otimes \hat{\mathbf{e}}$, $|\mathbf{e}| = |\hat{\mathbf{e}}| = 1$, $\mathbf{e} \cdot \hat{\mathbf{e}} = 0$, and
   (a) $\hat{\mathbf{t}} = \tau_1\mathbf{e} + \tau(\mathbf{e} \times \hat{\mathbf{e}})$, $\mathbf{t} = \tau_2\hat{\mathbf{e}} + \tau(\mathbf{e} \times \hat{\mathbf{e}})$ for some τ_1, τ_2, τ.

Reconstructed positions and orientations:

$$\begin{aligned} \mathbf{R}_{i+1,j+1} &= \mathbf{R}_{1,1}\mathbf{Q}^i\hat{\mathbf{Q}}^j, \\ \mathbf{y}_{i+1,j+1} &= \mathbf{y}_{1,1} + \mathbf{R}_{1,1}\left[\sum_{k=0}^{j-1}\hat{\mathbf{Q}}^k\hat{\mathbf{t}} + \hat{\mathbf{Q}}^j\sum_{k=0}^{i-1}\mathbf{Q}^k\mathbf{t}\right] \\ & i = 1, \ldots, N, \quad j = 1, \ldots, M. \end{aligned}$$

Precisely the formula for T4 tail sheath

Generic fully relaxed state

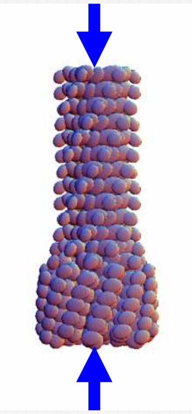


Helices in every rational direction of Z^2

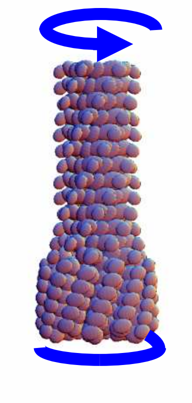
Force and moment at transformation

$$
\begin{aligned}
f &= f_{trans} = \frac{(\phi_c(\rho^e,\gamma^e) - \phi_c(\rho^c,\gamma^c))\lambda_c}{(\lambda^e - \lambda^c)} \\
&= \frac{(\phi_c(\rho_e,\gamma_e) - \phi_c(\rho_c,\gamma_c))}{(\frac{\lambda_e}{\lambda_c} - 1)} + \mathrm{O}\left(\max_{c,e} \frac{A_{c,e}}{A_{c,e}C_{c,e} - B_{c,e}^2} f^2\right)
\end{aligned}
$$

$$f_{trans} \doteq 103 \text{ pN}$$



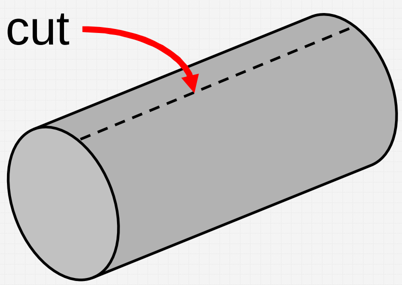
$$
\begin{aligned}
M &= M_{trans} = \frac{(\phi_c(\rho^e,\gamma^e) - \phi_c(\rho^c,\gamma^c))\lambda_c}{(\gamma^e - \gamma^c)} \\
&= \frac{(\phi_c(\rho_e,\gamma_e) - \phi_c(\rho_c,\gamma_c)))\lambda_c}{\gamma_e - \gamma_c} + \mathrm{O}\left(\max_{c,e} \frac{A_{c,e}}{A_{c,e}C_{c,e} - B_{c,e}^2} M^2\right)
\end{aligned}
$$



$$f_{trans} \approx \frac{\gamma_e - \gamma_c}{\lambda_e - \lambda_c} M_{trans} = -\frac{1}{89 \text{ Å}} M_{trans}$$

Unrolling, interfaces

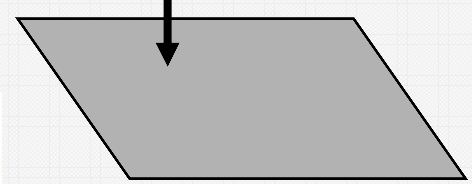
One can cut tail sheath on a generator and unroll, without violating the constraints.



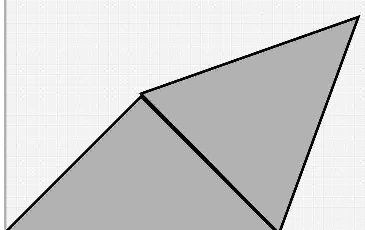
unroll

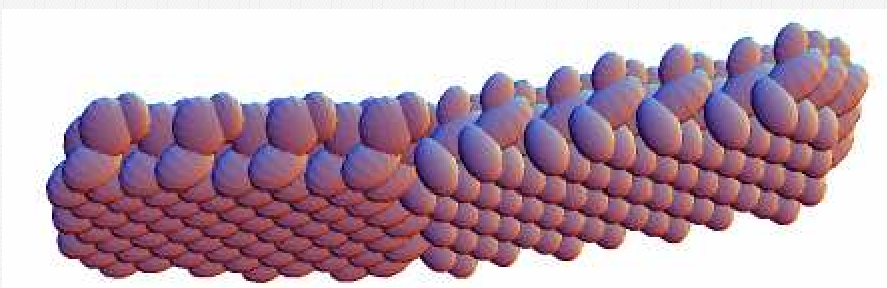
$$\mathbf{F} = \begin{pmatrix} 0.053 & -1.088 \\ 0.999 & 1.543 \end{pmatrix}$$

transform

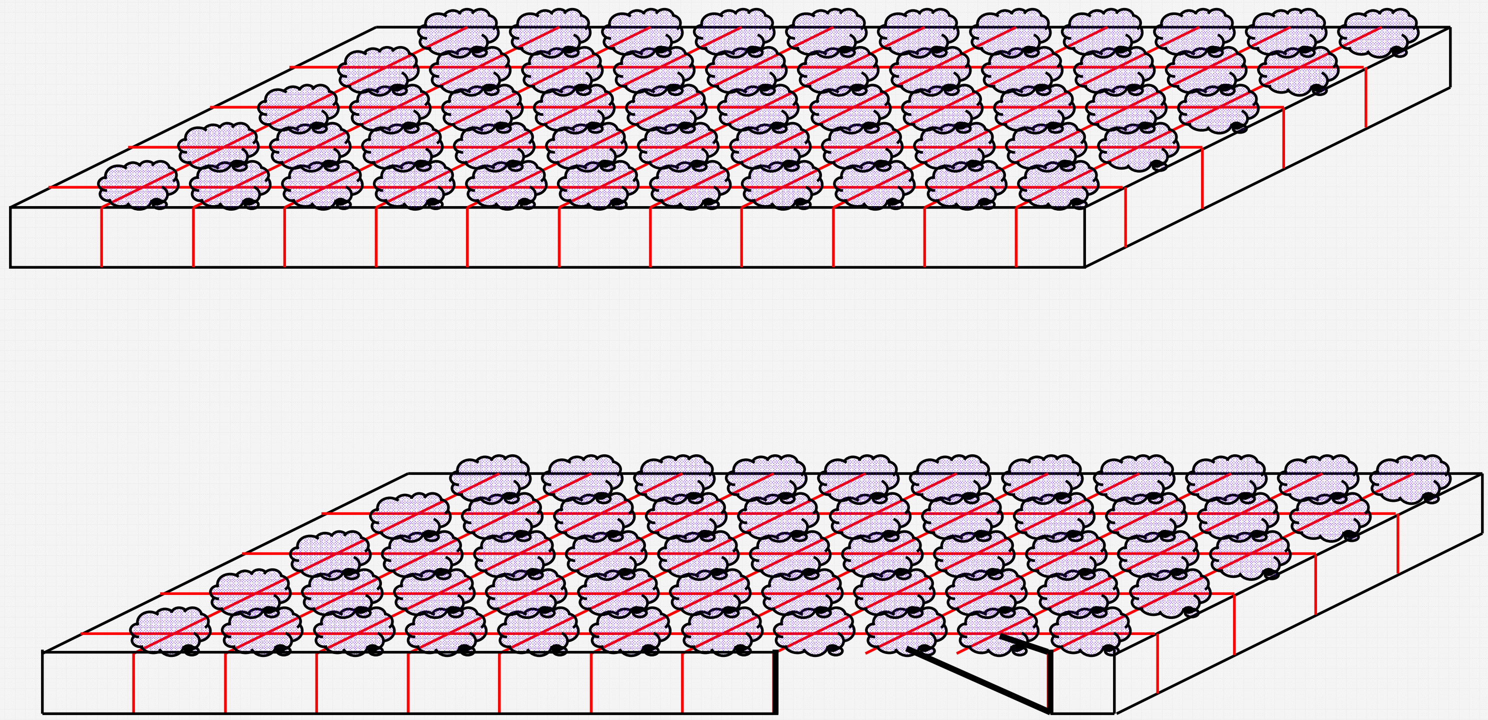


F has eigenvalues 0.567 < 2.06



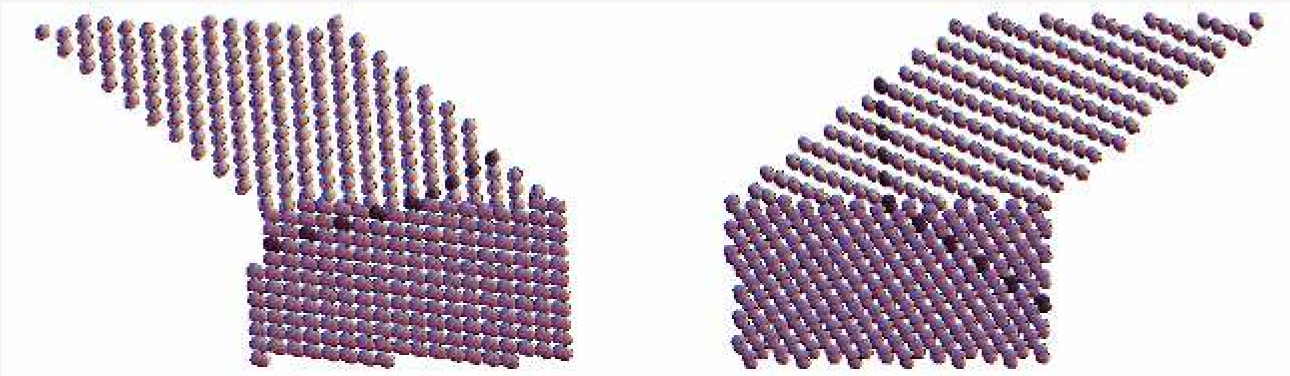


Bio-Molecular Epitaxy (BME)

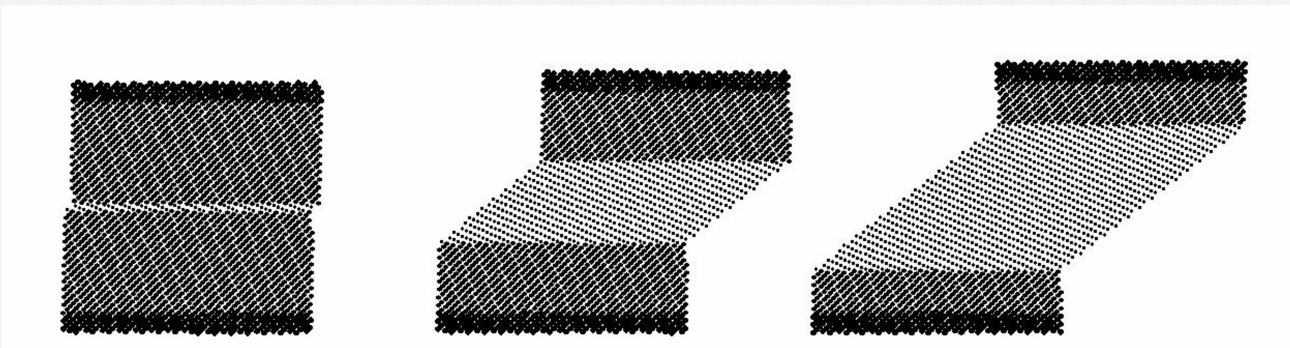


Patterning

The two interfaces in the unrolled sheet:



A patterning strategy:



Suggestion for producing an actuator that interacts intimately with biology, made of proteins

- Biomolecular epitaxy
  - Lots of flexibility: molecule shape, solution chemistry
- Develop patterning strategy
- Test mechanical behavior
- Build mathematical theory

Falk, W. and R. D. James, An elasticity theory for self-assembled protein lattices with application to the martensitic phase transition in bacteriophage T4 tail sheath, *Phys. Rev. E* (2005), submitted.