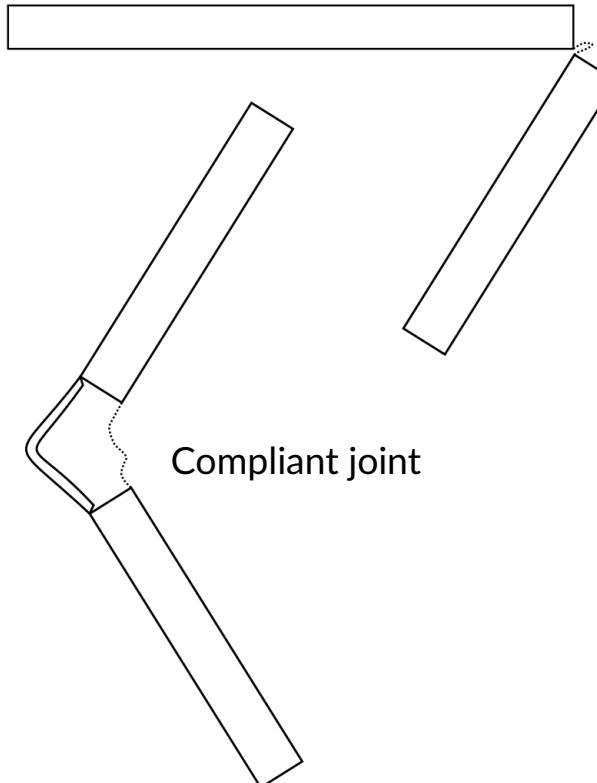
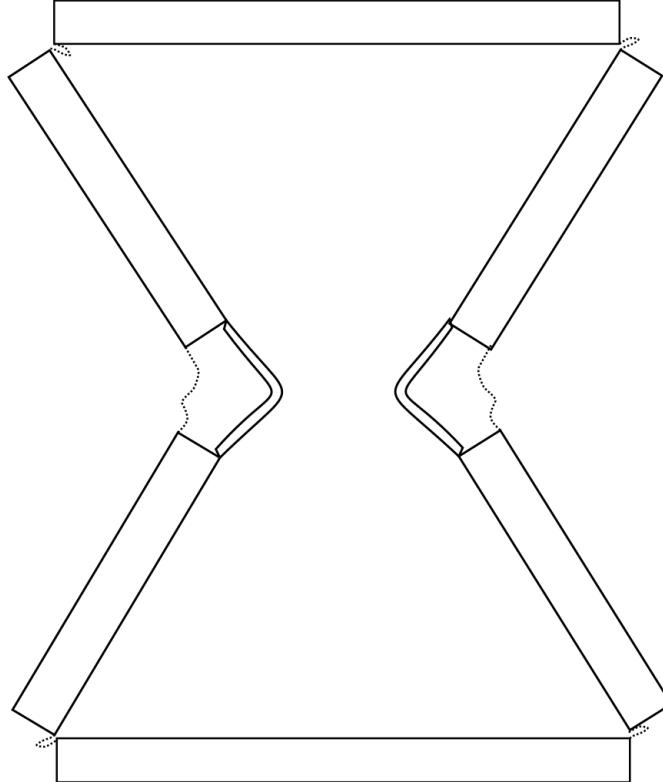
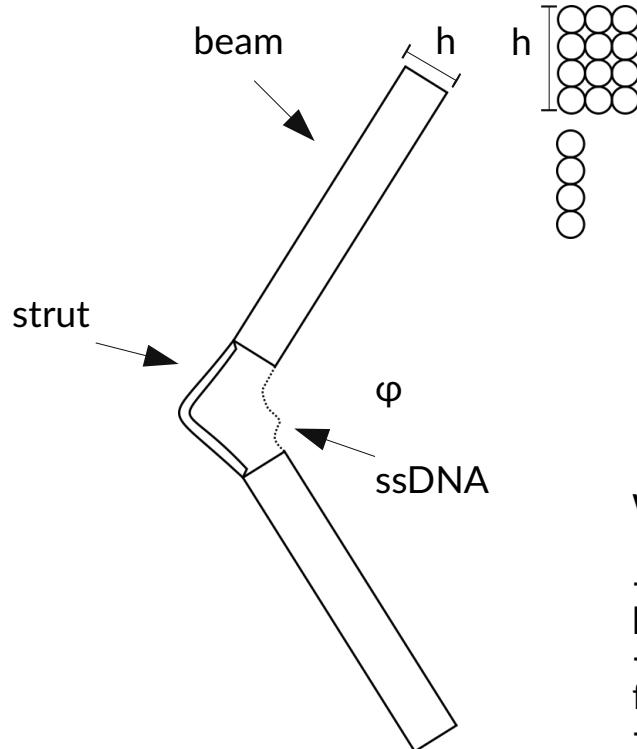


Honeycomb monomer



Reentrant honeycomb monomer consists of two mechanical linkages

Compliant Joint



Compliant joint uses balance of energies between ssDNA and bendable strut to induce bending at desired angle.
Use square design grid rather than honeycomb for ease of description.

Degrees of freedom:

- strut cross section
- strut length
- ssDNA length
- beam cross section.

We want to minimize scaffold:

- strut can be 2x1, 4x1, 6x1 etc (must be even for Eulerian graph)
- strut length must be long enough for a few internal crossovers
- beam cross section can be 4x3, 4x4 etc (can't do 4x2 because not enough moment generated by ssDNA then.)

Choose these design parameters:

- strut is 4x1 as must have a few crossovers, and be small
- Use 30 bp, and 40 bp; 30 bp is probably too short...
- Use beam cross section 4x3 as otherwise don't have enough scaffold

Lifeng Zhou, Alexander E. Marras, Carlos E. Castro, and Hai-Jun Su

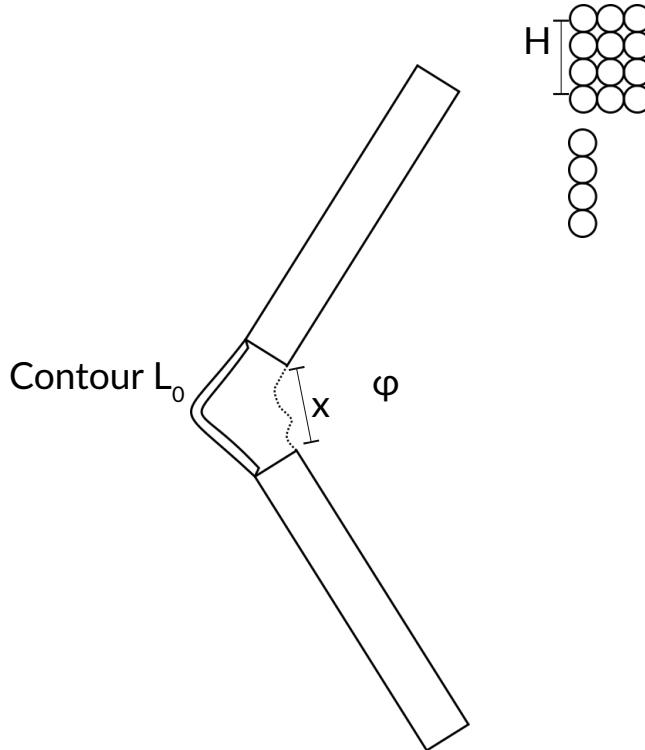
Department of Mechanical and Aerospace Engineering

The Ohio State University

Columbus, Ohio, USA

Email: zhou.809, marras.3, castro.39, su.298@osu.edu (corresponding author)

Analytical Description



We want to evaluate bending angle:

(1) Energy from beam deformation.

→ Get Young's modulus of DNA from $E_{dsDNA} = L_p k_B T / I_{dsDNA}$
persistence length

→ Get second moment of DNA from $I_{dsDNA} = \pi^2 D^4 / 64$
imagining it's a solid cylinder

→ Get beam stiffness (c is empirical
correction factor)

→ Get energy in beam

$$K = cEI/L$$

$$E_{beam} = \frac{1}{2} K(\pi - \phi)^2$$

(2) (Free) energy from ssDNA

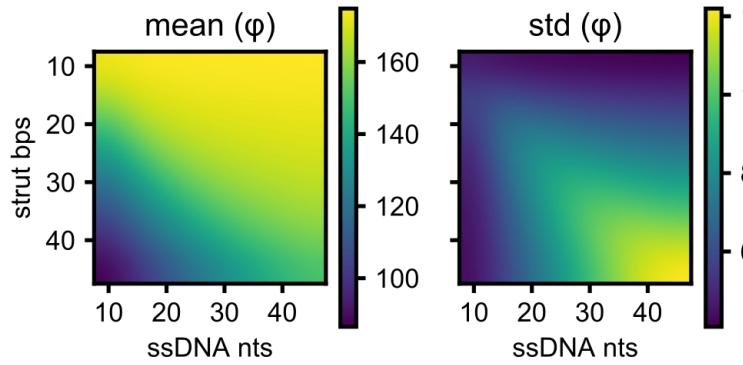
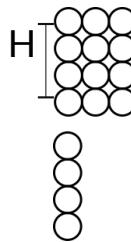
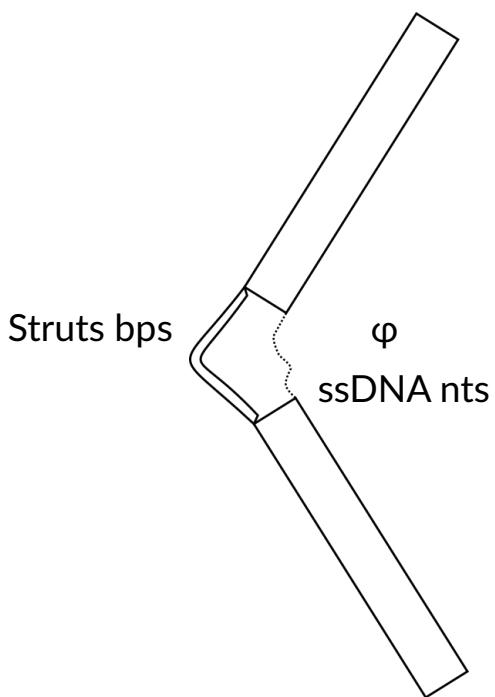
→ Treat as power expansion of WLC

→ Persistence length L_p , with contour length L_c .
 $G_{WLC} \approx \int_0^x dx \cdot \frac{k_B T}{L_p} \left[\frac{1}{4(1-x/L_c)^2} - \frac{1}{4} + \frac{2}{L_c} \right]$

Combine estimates to get total free
energy as a function of bending angle.

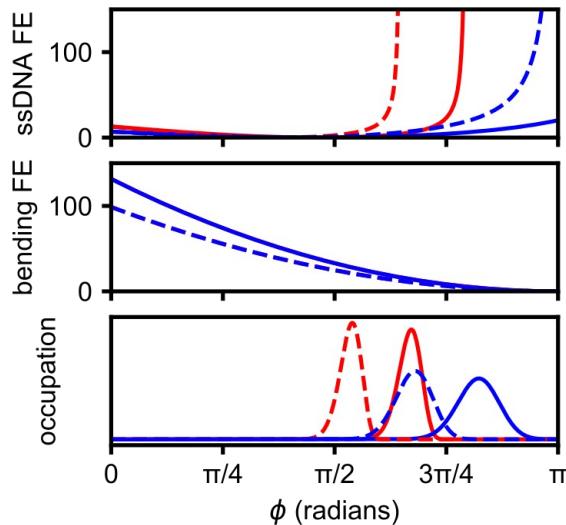
$$G = E_{beam} + G_{ssDNA} \cdot N_{ssDNA}$$

Analytical Results



Big strut length L_0 means narrow angle. Lots of ssDNA means wide angle.

In general, a big strut, and lots of single stranded DNA mean a wider angle distribution.

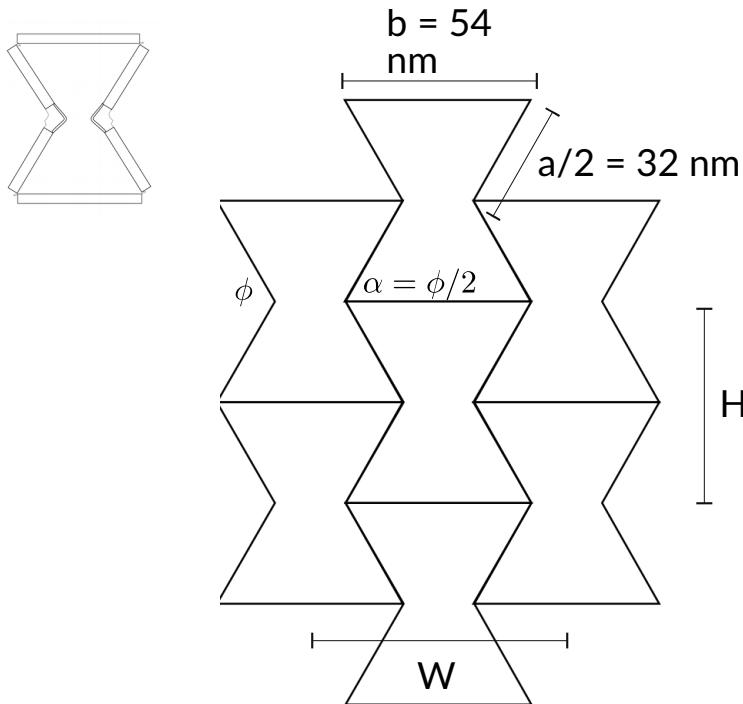


Free energy contributions (units are in $k_B T$). Occupation is the negative exponential of sum of free energies; very close to normal distributions: think power expansion of distribution at minimum. Implies angle distribution can be described well by harmonic potential.

Constitutive relationship of a material with unconventional Poisson's ratio

TEIK-CHENG LIM

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Analytical treatment of honeycomb

What does the angular potential mean for material Poisson ratio and stiffness? Model geometrically. We abstract system to honeycomb network with angular potential, forgetting about implementation details.

We want to evaluate Poisson ratio. Poisson ratio is (highly) anisotropic, so look at ratio of horizon strain (in W) to vertical strain (in H).

Constitutive equation governs stress / strain. Elements are kind of like (2D stiffness). Elements are multiplied by stiffness parameter.

Elements then become:

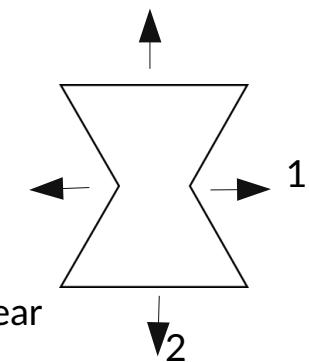
$$\nu_{12} = -\frac{\sin \alpha \tan \alpha}{2b/a - \cos \alpha}$$

$$K = 2k_\theta/V_0$$

$$\sigma_1 = C_{11}\epsilon_1 + C_{12}\epsilon_2$$

$$\sigma_2 = C_{11}\epsilon_1 + C_{22}\epsilon_2$$

$$\tau_{12} = C_{33}\gamma_{12}$$



$$C_{11}/K = \left[\frac{2b/a}{\sin \theta} - \frac{1}{\tan \theta} \right]^2$$

$$C_{12}/K = \frac{b/a}{\cos \theta} - \frac{1}{2}$$

$$C_{22}/K = \tan^2 \theta$$

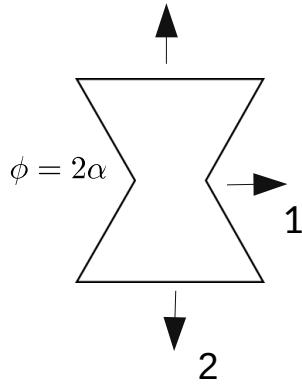
How hard to widen?

How hard to lengthen?

$$C_{33}/K = \left[1 - \frac{\cos \theta}{2(b/a)} \right]^2$$

How hard to shear?

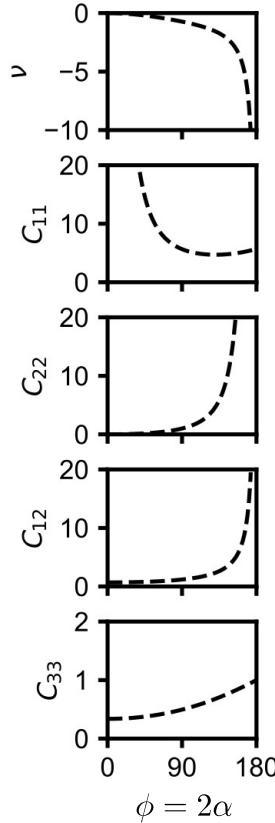
Analytical treatment of honeycomb



$$C_{11}/K = \left[\frac{2b/a}{\sin \theta} - \frac{1}{\tan \theta} \right]^2$$

$$C_{12}/K = \frac{b/a}{\cos \theta} - \frac{1}{2}$$

$$C_{22}/K = \tan^2 \theta$$



(-) fractional increase in width per fractional increase in height.

How hard to widen?

How hard to lengthen?

How hard to widen by pulling vertically.

How hard to shear?

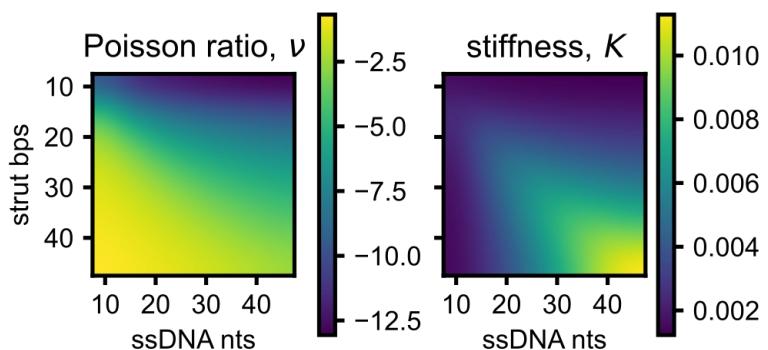
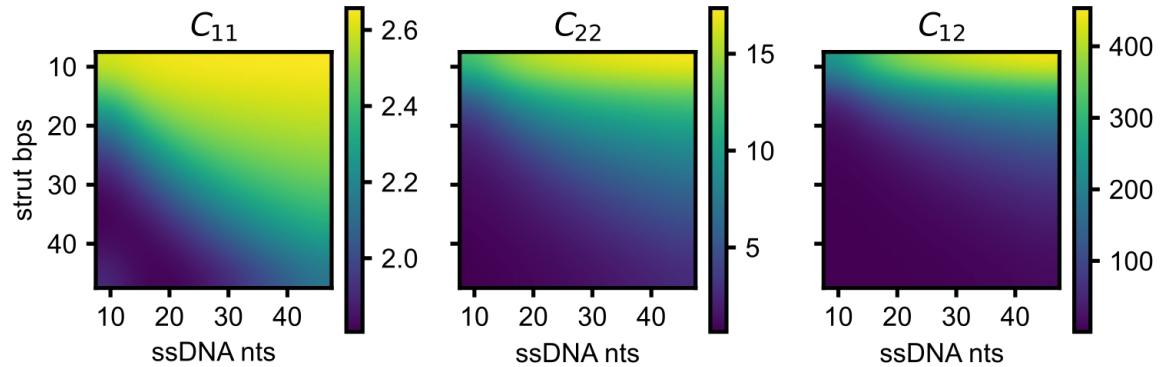
Various physical quantities diverge, including the Poisson ratio.

C_{22} diverge because no matter how hard you pull vertically (2), you're not going to be able to cause the system to get taller if the bending angle is close to 180 (i.e. hourglass \rightarrow rectangle).

C_{12} diverges because no matter how hard you pull in direction (2), you're not going to be able to make the system get wider than a rectangle ($\phi \rightarrow 180$).

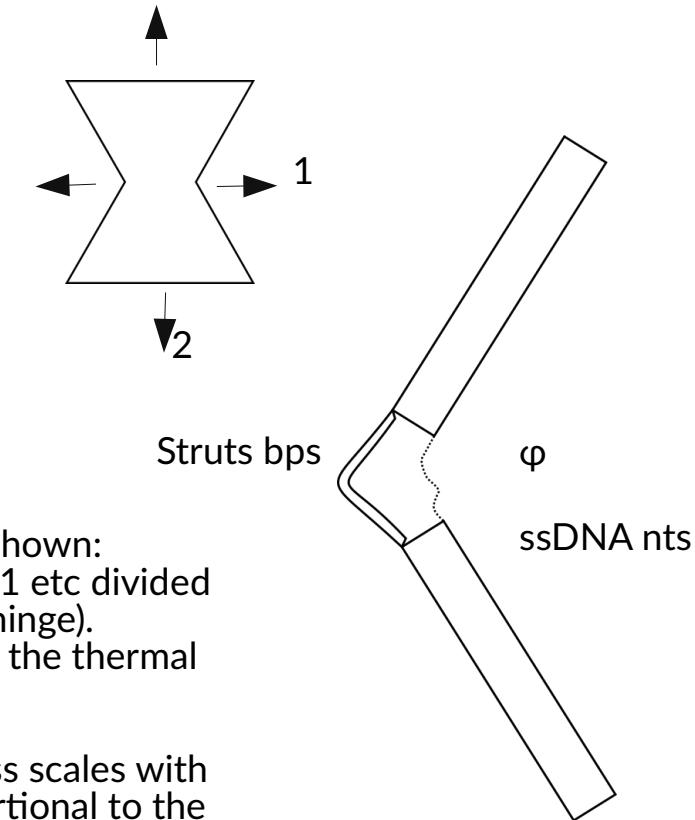
v_{12} as described here is the ratio of horizontal strain to vertical strain. At $\phi = 180$, the derivative of height wrt ϕ is 0, but the derivative of width wrt ϕ is not 0. Therefore v_{12} diverges (while v_{21} is 0 here, as the two Poisson ratios are inverses).

What would the parameters of our material be?

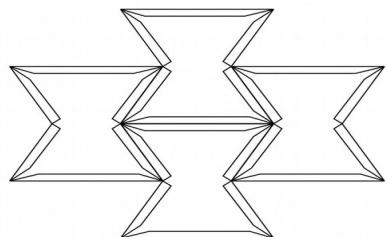
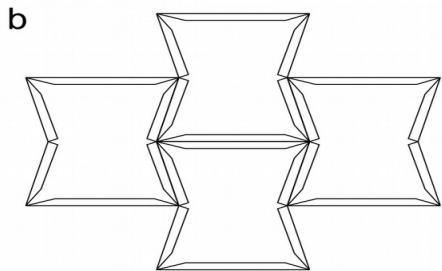
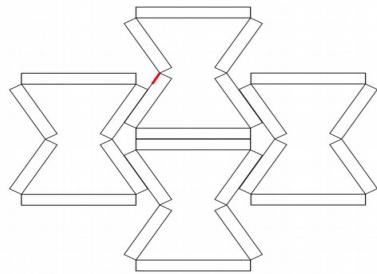
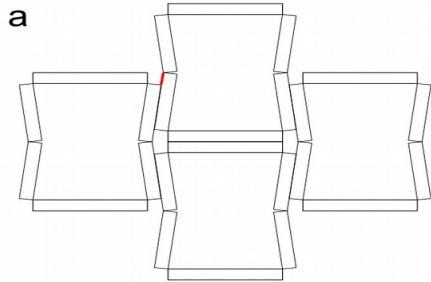


Various geometrical stiffnesses shown:
(geometrical stiffness \rightarrow True C_{11} etc divided by K , which is a property of the hinge).
Haven't put units... will work out the thermal occupation later.

Value of K also shown. K stiffness scales with angular stiffness, which is proportional to the inverse variance of the angular distribution;
so distribution looks familiar...



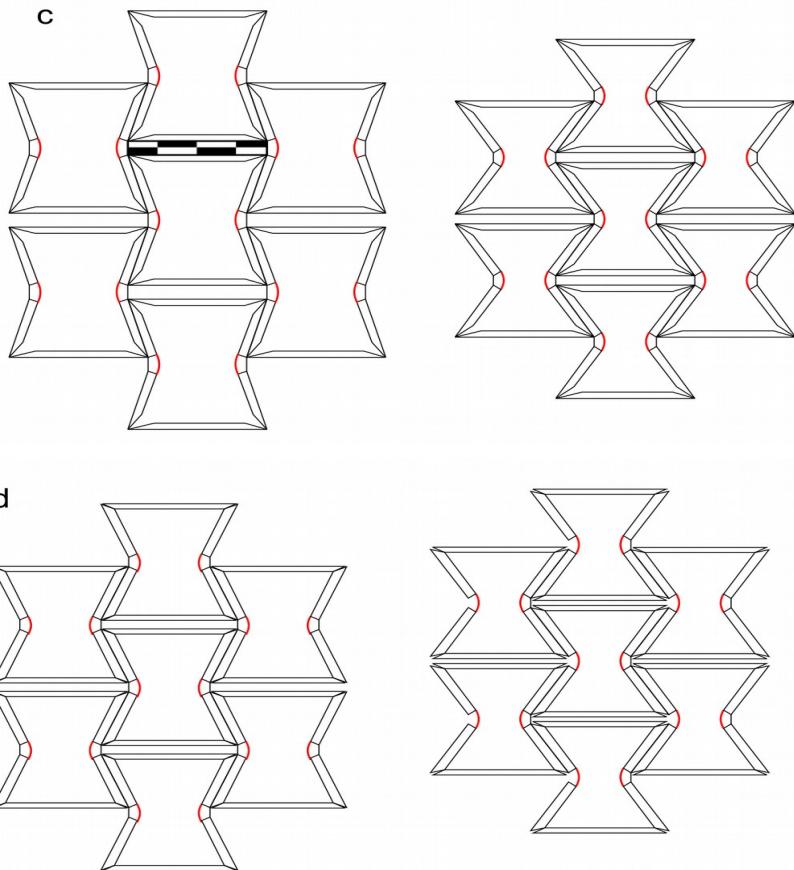
How can we polymerize?



(a) Finite thickness re-entrant honeycomb monomers forming a 2d material need to slide along each other for deformation to happen. The red line is the same length in both left and right. This sliding is bad as we can't encode sliding constraints in DNA.

(b) If connections are made at the outer vertex of all beams, then deformation without sliding is possible. However, this model of the hinge isn't realistic.

How can we polymerize?

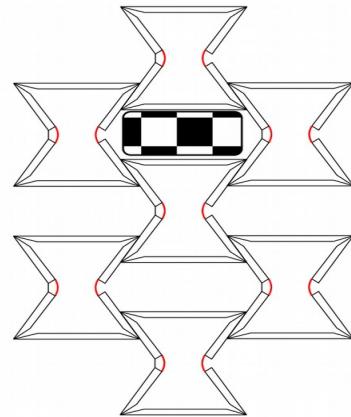
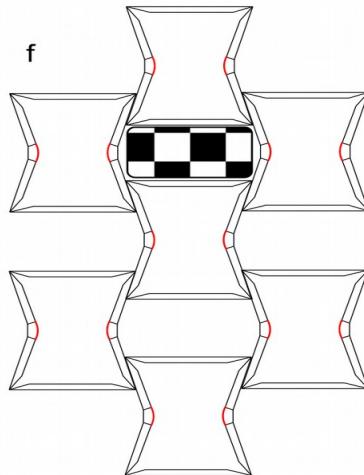
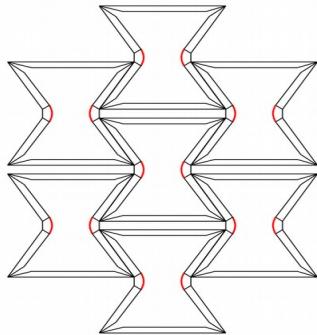
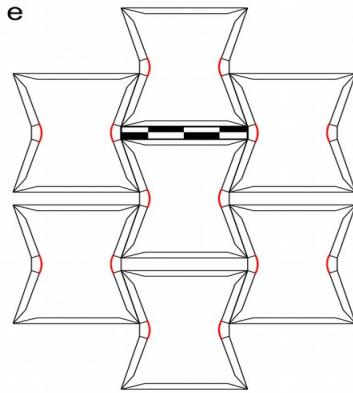


(c) deformation without sliding becomes possible for our non ideal joints if each origami monomer has 4 rather than 6 connections with other origami.

This leaves a void (checkerboard) between adjacent (north-south) monomers.

(d) If we accept that each origami monomer need only have four nearest neighbours then our requirement that all beams be joined via the outside edges is relaxed. Here I have jointed beams via their inside edges as an example (this is the origami I simulate in subsequent slides).

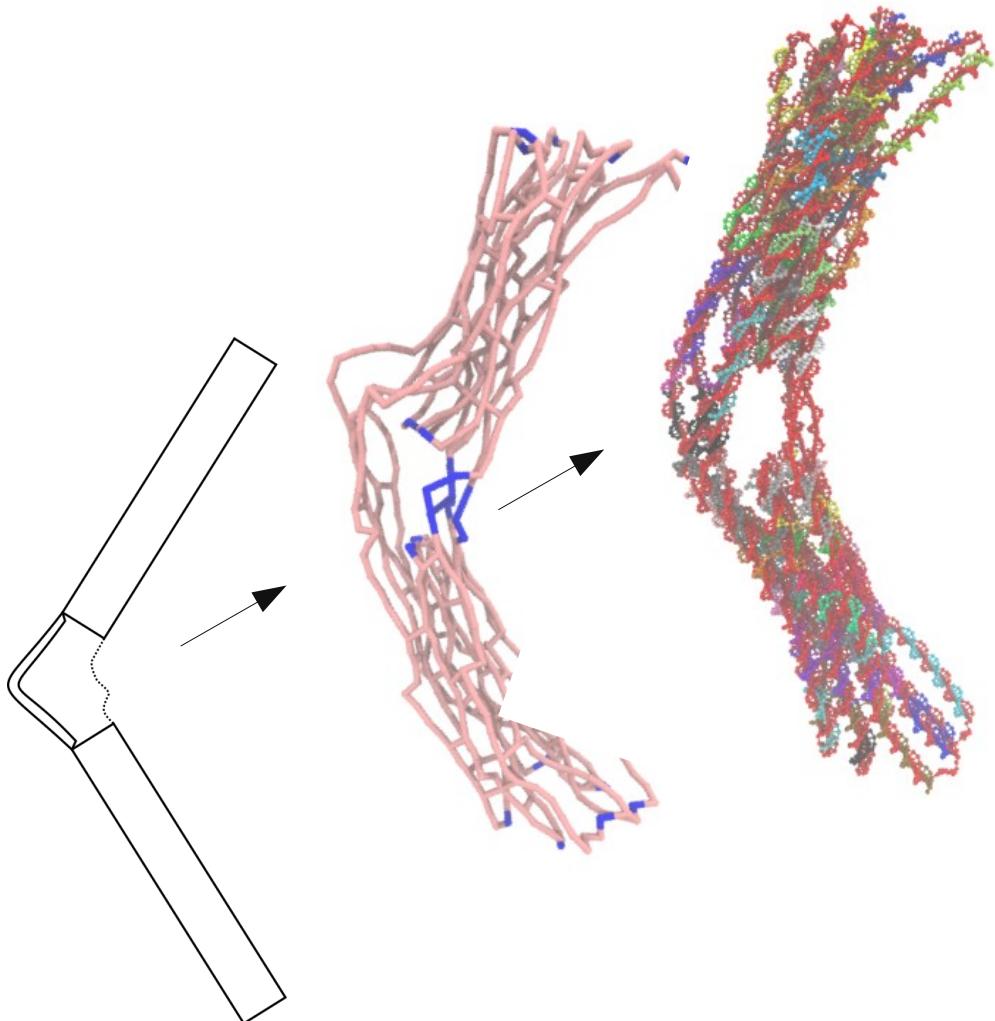
How can we polymerize?



Since each origami now has four connections instead of six, we have increased freedom in how origami are attached. (e) demonstrates an attachment where origami bind along the entire length of their beams.

(f) indicates binding via approximately half of the beam length, resulting in an increased size of void. In principle this may provide a further parameter with which to tune material properties, although I haven't gone through the maths yet.

Simulation



Objective: get angular distributions in oxDNA and look for non-idealities our very coarse-grained analytical description has missed.

Difficulty: relaxation to equilibrium in oxDNA takes ages.

Therefore I design structures in MagicDNA, and export them in an oxDNA format.

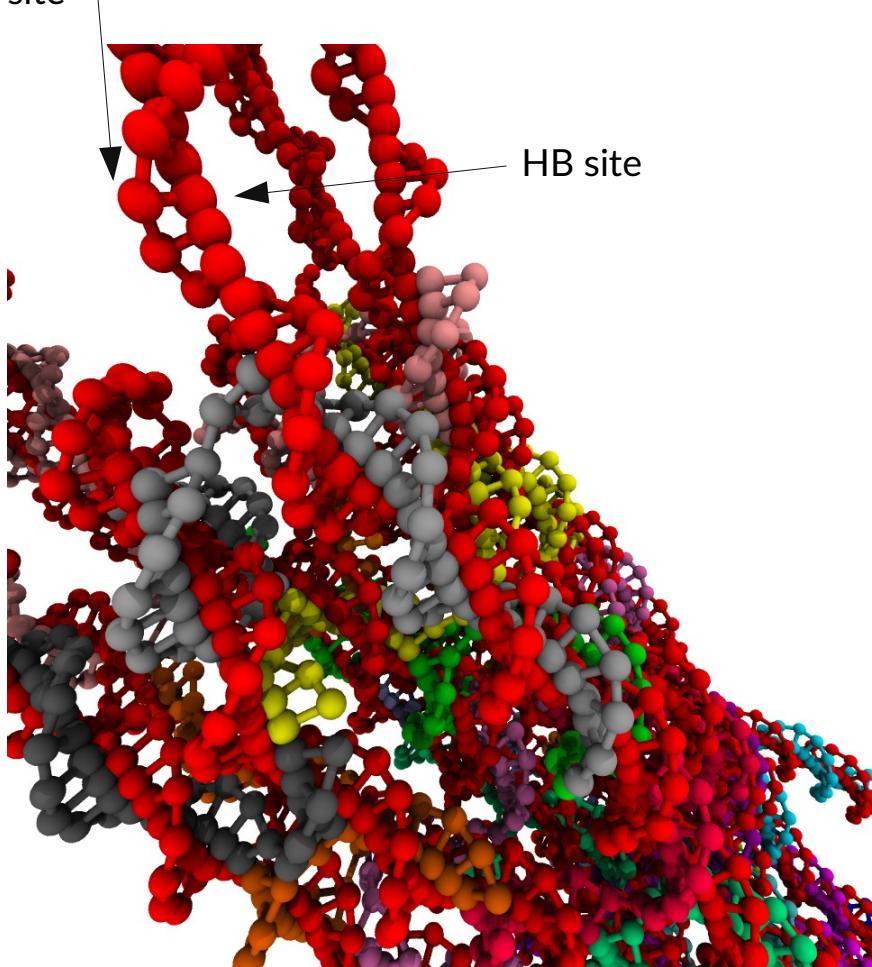
I wrote an oxDNA -> mrDNA converter which generates mrDNA structures from oxDNA structures (this wasn't trivial... I needed to use some clever datastructures to make this time and space efficient. I'll write it up and put a link on the oxDNA slack).

I then simulate in mrDNA (using a GPU) for about 1×10^7 timesteps using 5 bp per bead, then for an additional 1×10^7 timesteps using 1 nucleotide per bead with explicit twist.

These relaxed structures are then converted to oxDNA structures and we run for approximately 100 ns of simulation time (40 hours).

phosphate
repulsion
site

New oxDNA visualization tool



All of the oxDNA visualization tools are kind of terrible. This has annoyed me for a while, and I feel like there's lots of interesting information we're missing out on because we can't see it.

- (1) UCSF Chimera is slow and doesn't really see trajectories
- (2) Cogli1 (the one Lorenzo wrote) is cool but a bit amateurish, and slow
- (3) oxdna-viewer is basically not extensible because it's written in Javascript, and also it's new so rendering is difficult, and doesn't have the features older things have.

I wrote a few scripts that let you see oxDNA structures nicely in VMD, with bond connectivity / individual strand / index query functional. Locations of stacking sites also visible.

I also created some scripts that can color code nucleotides by various types of energy, which is cool, so you can directly visualize the distribution of "molecular strain" (see later). You can see which nucleotides are strained / which are stacked / which are bonded on average.

WillTKaufhold1/will_oxdri x how to buy a fox - Google x cute fox pictures - Google x +

github.com/WillTKaufhold1/will_oxdna_vmd

Apps ori netflix https://raw.gi... localhost:3000 Lab Streaming... GitHub - lohed...

WillTKaufhold added image descriptions Latest commit 673e6da 14 seconds ago

images	changed some ppm into png	13 minutes ago
src	first commit	2 hours ago
.README.md.swp	added image descriptions	14 seconds ago
LICENSE	Initial commit	2 hours ago
README.md	added image descriptions	14 seconds ago

README.md

Will's oxDNA scripts for VMD

Intro

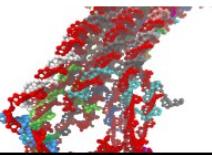
I wanted to integrate oxDNA effectively into VMD. These are a collection of scripts that perform this integration. The reason I wanted effective integration was that I wanted to lever the VMD package ecosystem when analysing DNA origami.

The scripts here take an oxDNA.dat file, and generate a .xyz file, and a .psf file. Locations of hydrogen bonding (HB) and phosphate repulsion (BB) sites are placed in the .xyz file, and bond connectivity is placed in the .psf file. Bond connectivity includes one bond between the HB site and BB site, and a second bond between BB sites that are connected.

There are also scripts here that extract energy profiles from simulation trajectories, and then colorcode nucleotides in VMD according to energy value. Specifically nucleotides can be colored according to each the value of each energy component in the oxDNA force field. These components can be:

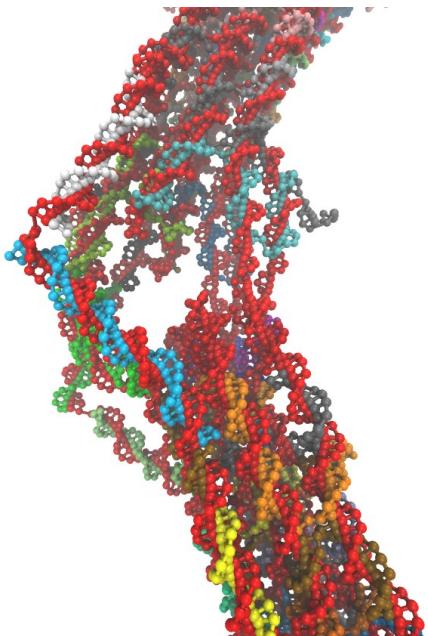
1. FENE : Finite extension non-linear elastic potential; backbone stretching.
2. BEXC
3. STCK: Stacking energies
4. NEXC: Excluded volume
5. HB: Hydrogen bonding
6. CRSTCK: Cross stacking
7. CXSTACK: Unused
8. DH:
9. total: total energy

Example rendered images

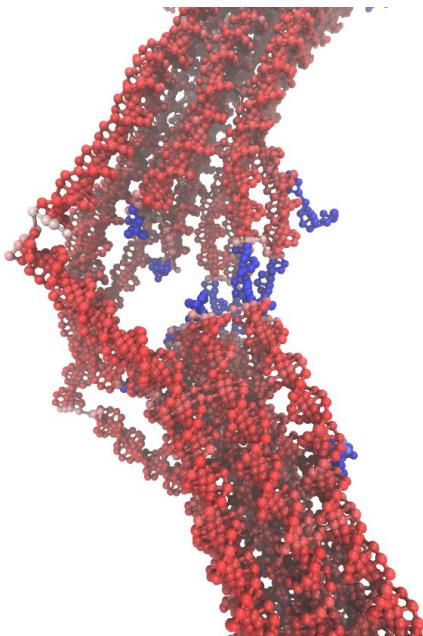


All of my scripts are online at
https://github.com/WillTKaufhold1/will_oxdna_vmd

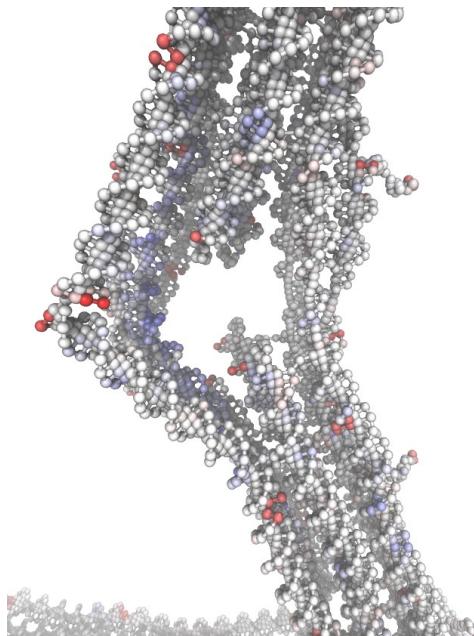
Seeing \langle energy \rangle is great for insight.



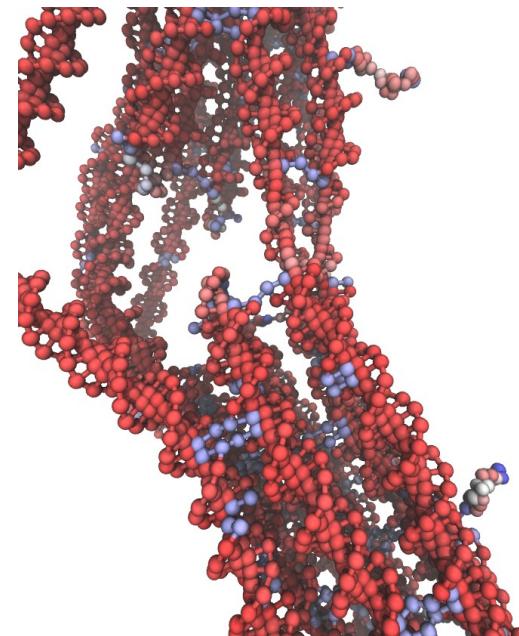
Strand identity



Hydrogen bonding



Backbone stretching



Stacking



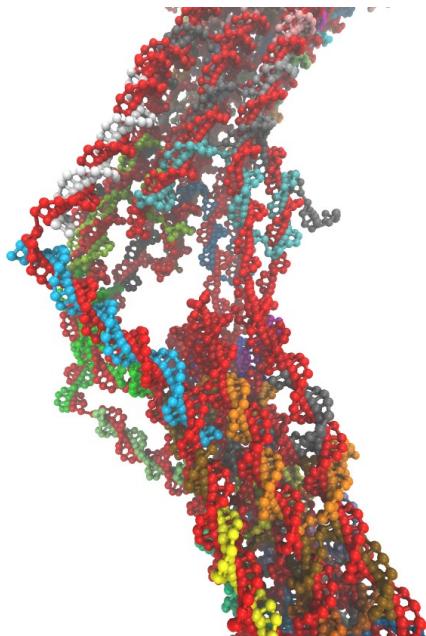
Favorable



Unfavorable



Have a look at these features



Strand identity

Hydrogen bonding

Backbone stretching

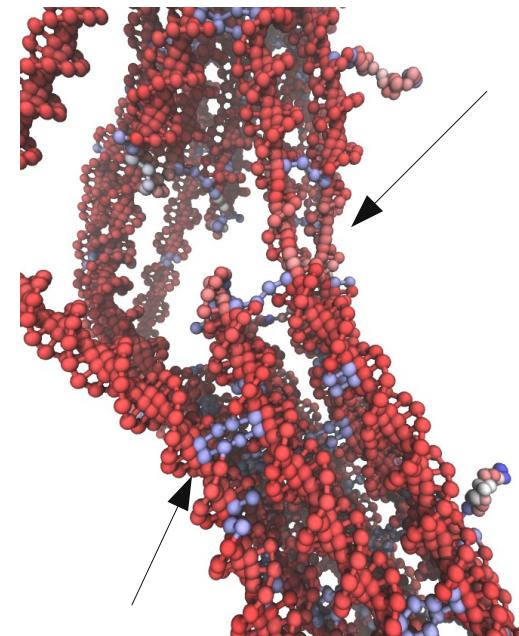
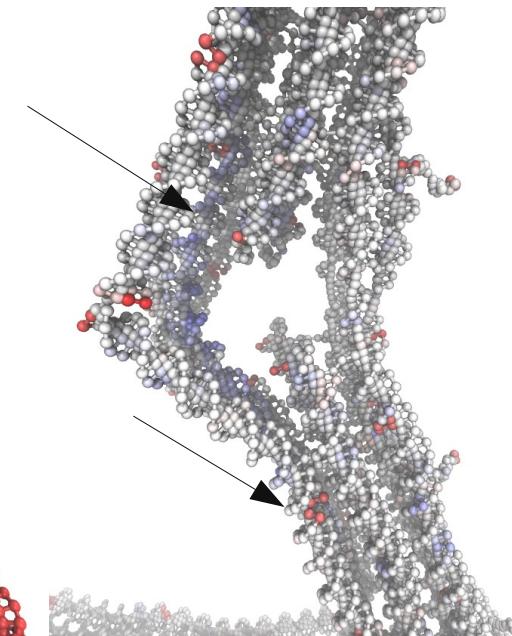
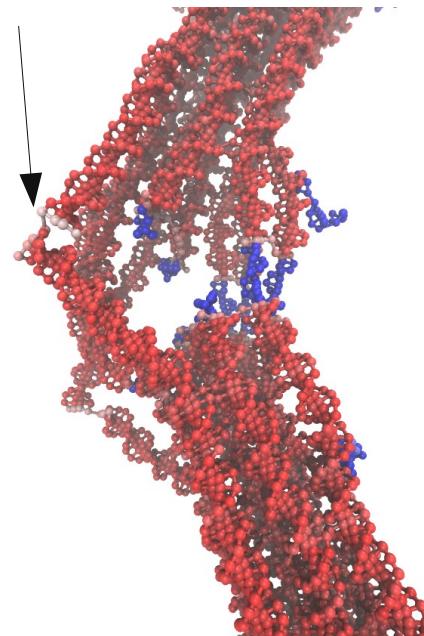
Stacking

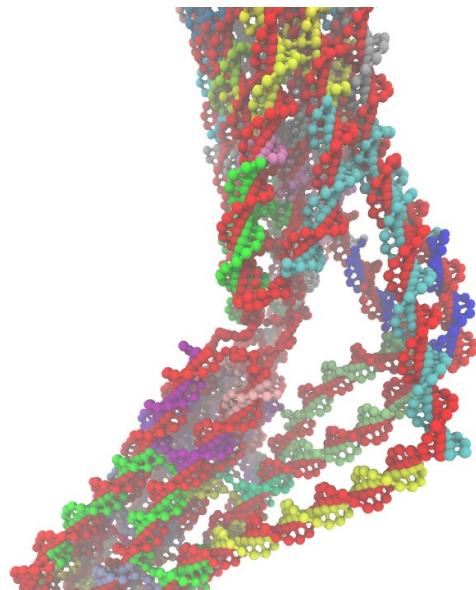
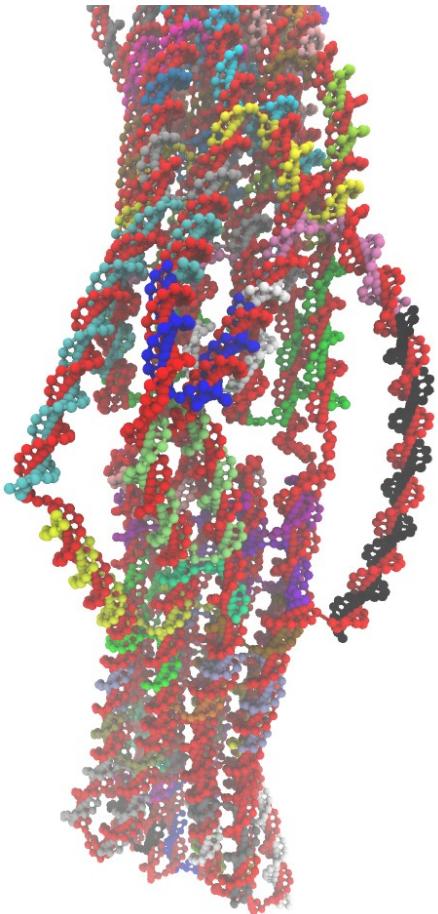


Favorable



Unfavorable





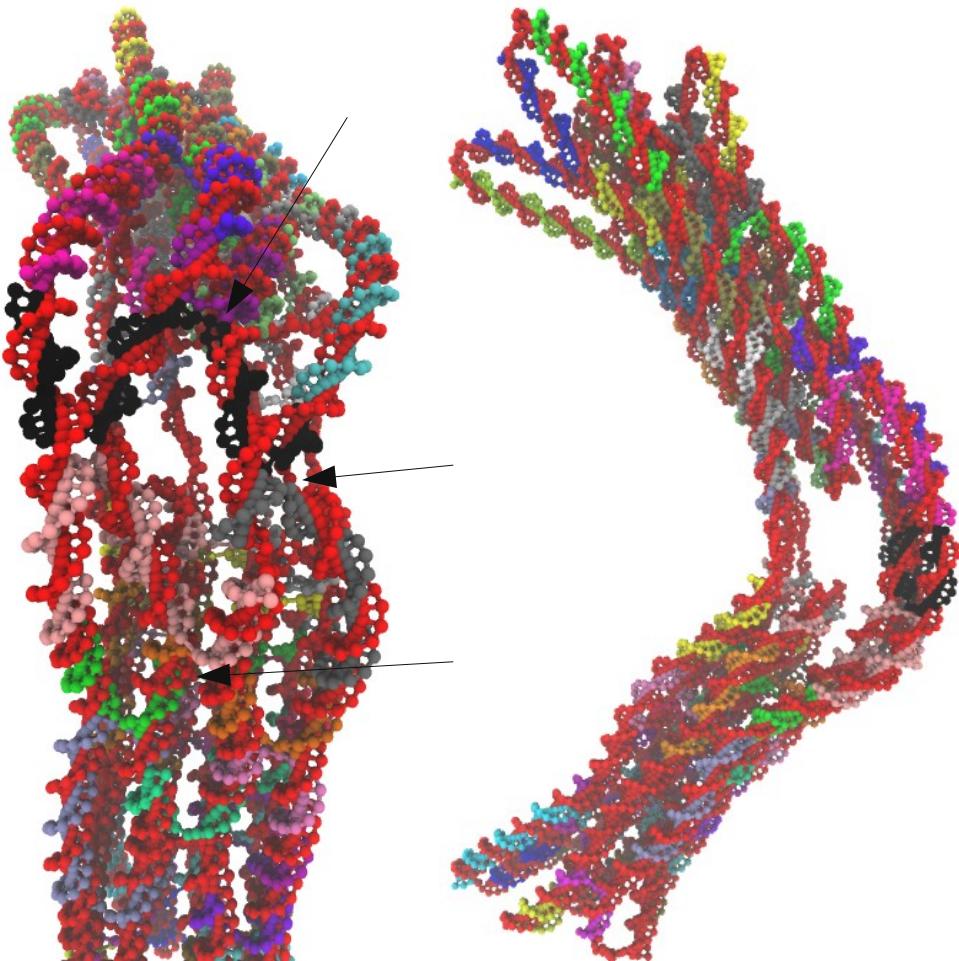
strut = 30 buckles

For the 4 x 1 strut, there is only one central crossover between the helices; the other two helices are effectively just normal WatsonCrick helices.

This is unable to withstand the torsion from the ssDNA, and several effects occur:

- (1) The outside helices unstack at the termination of the staples
- (2) The two inside helices unstack at the location of the crossover, which appears to be a weak point
- (3) The two outside helices "bow" out, so that their curvature decreases.

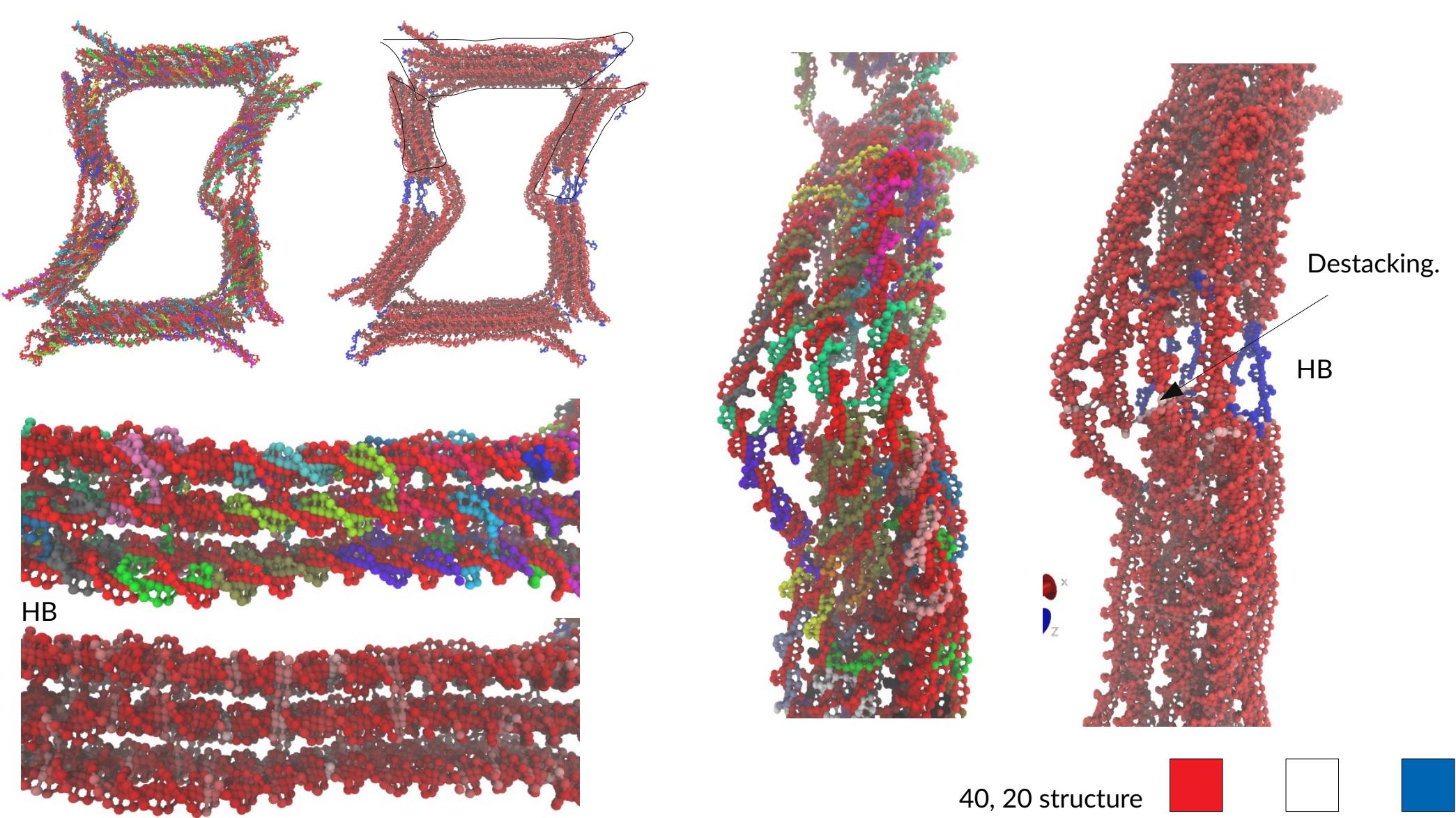
strut = 40 bends rather than buckling.

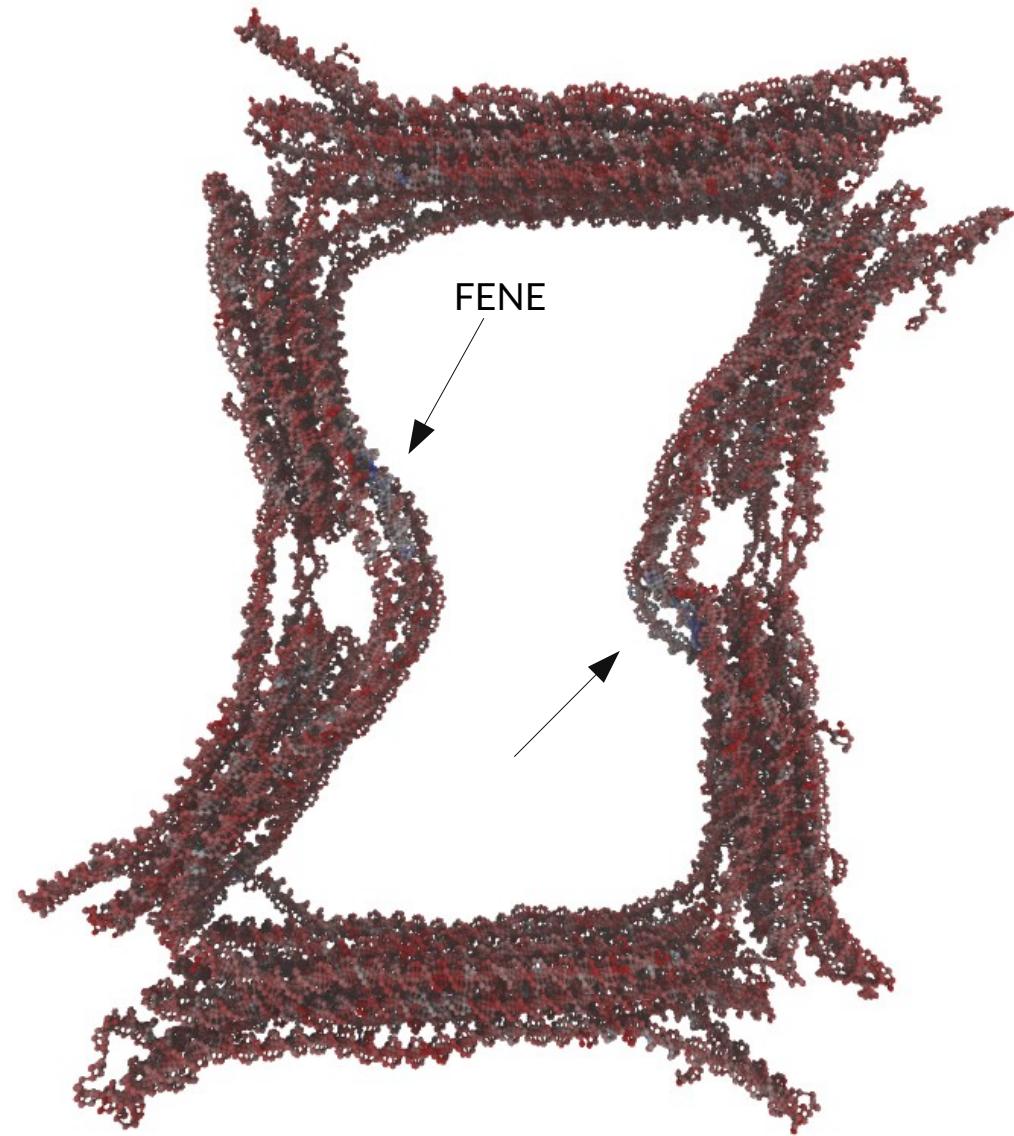


For the 4×1 strut, there are two outside crossovers (i.e. between the left two and the right two helices), and two inside crossovers (i.e. just between the two inner crossovers).

I would imagine that the multiple crossovers creates locations where strain can dissipate, so there's no need for dramatic unstacking events.

Would be very easy to do a systematic study of how crossover distribution affects buckling. (but let's not get even more distracted)



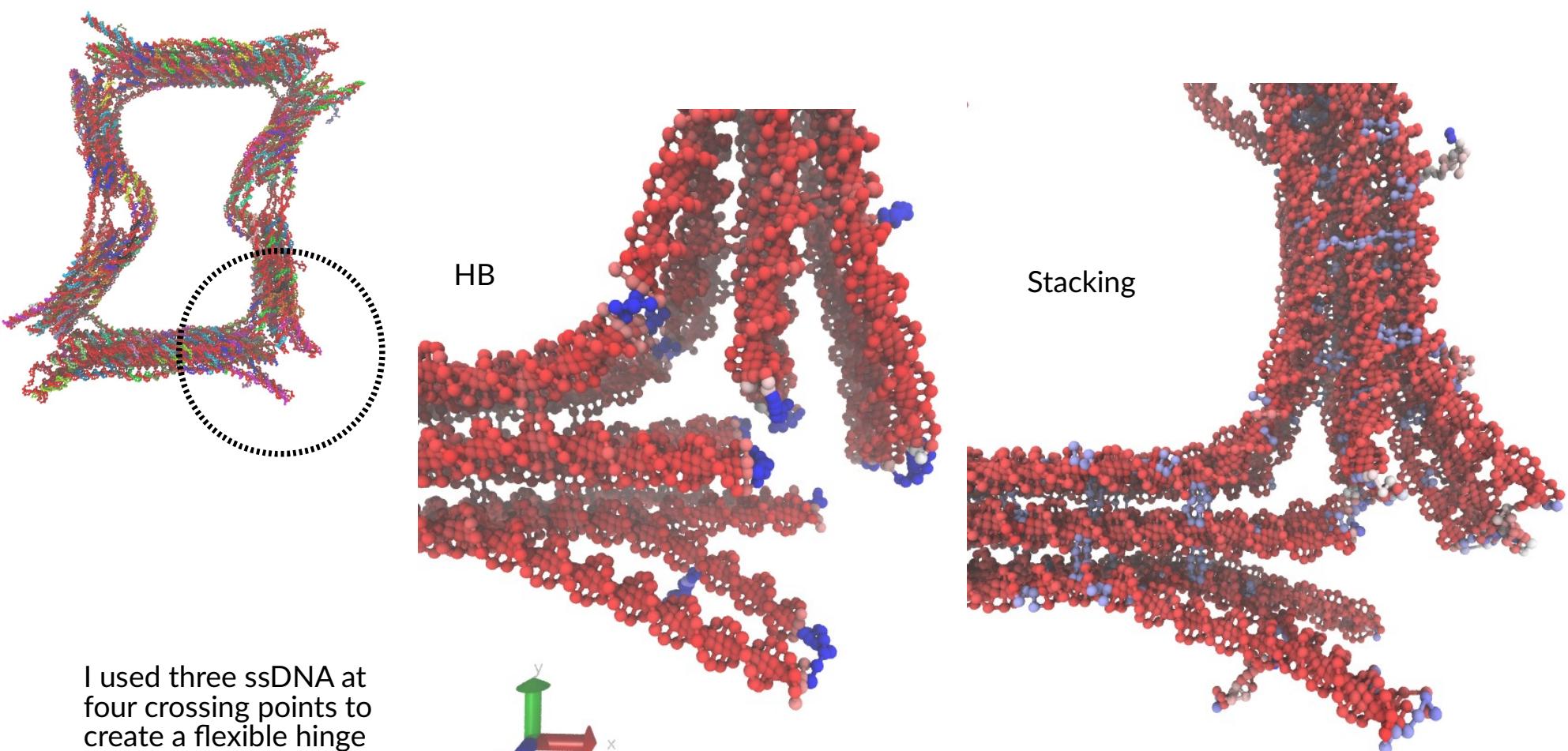


FENE energy distribution over compliant strut is very lopsided... our analytical model of the hinge imagines strain is distributed uniformly along it.

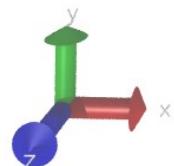
(N.B: FENE is the potential of the backbone connectivity; blue means overstretched or overcompressed backbone)

Notice also the entire hourglass is sheared a bit... non uniform FENE distribution over compliant joints probably linked to shear.

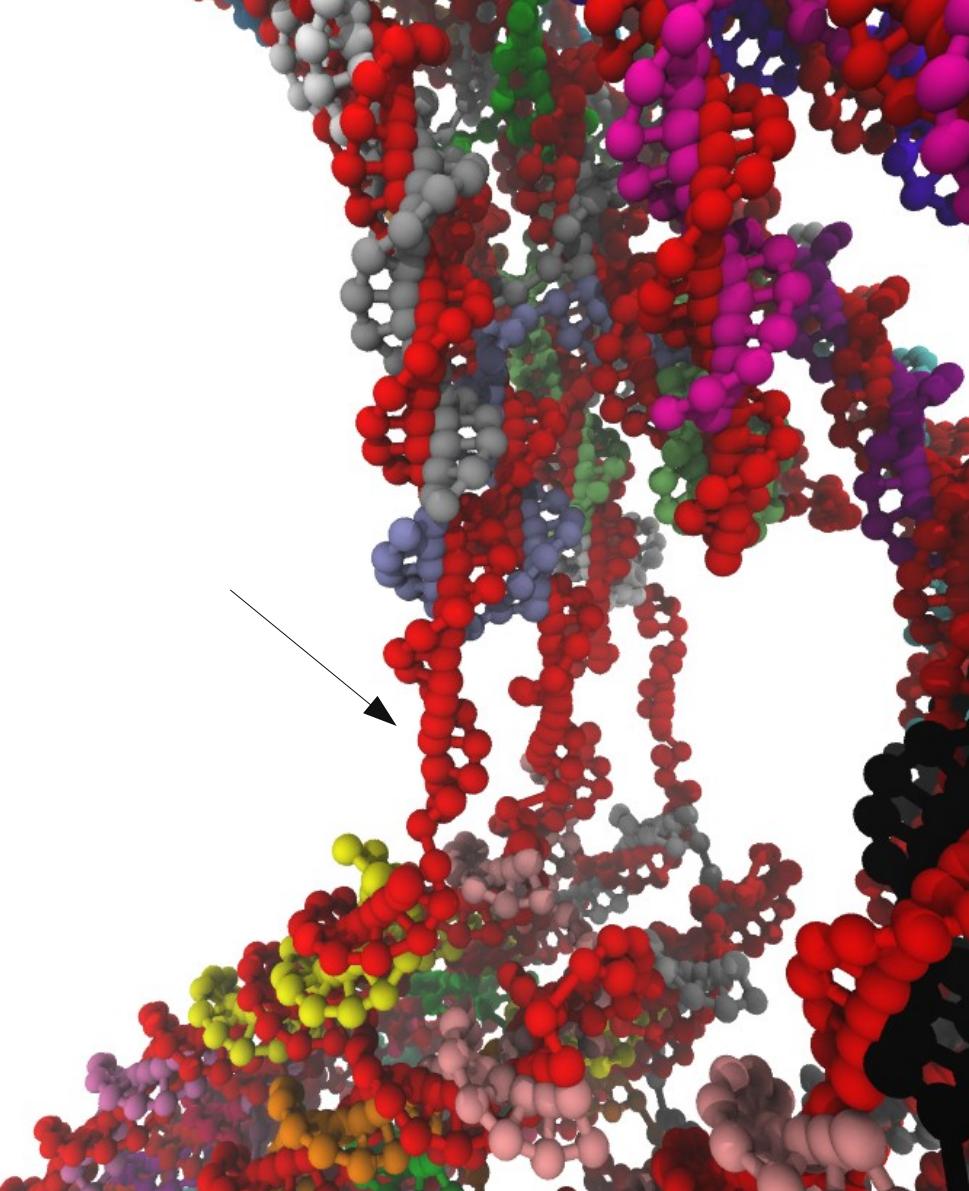
Interesting, and very weird.



I used three ssDNA at four crossing points to create a flexible hinge joint. However, we predict strong stacking at the joint; not really completely free to move.



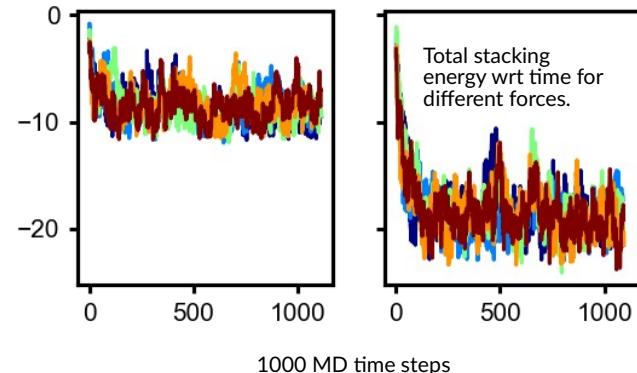
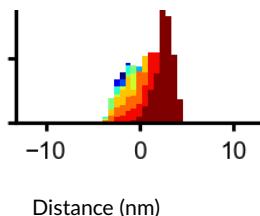
ssDNA in bridge is helical.



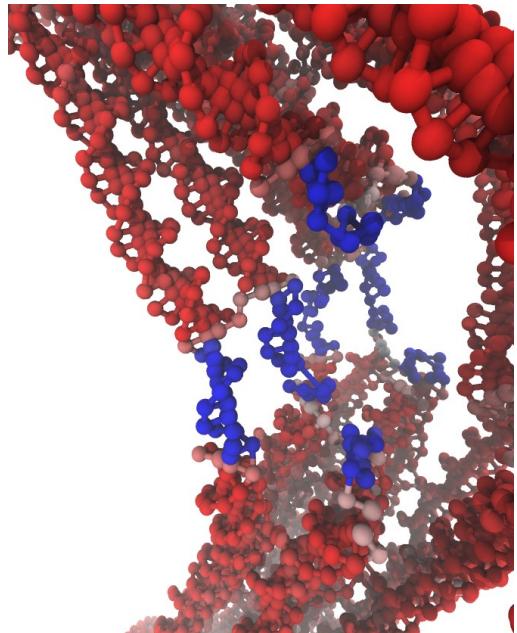
Is it obvious that single stranded DNA under tension becomes helical? I would have thought this should happen... if you tension a single strand of DNA, then you increase the energy of configurations which aren't colinear with the applied force.

So these states are occupied less, and the only states that are left are the stacked states... I tried to replicate this effect with explicit forces, but I can't. Maybe it's to do with stacking with the duplex?

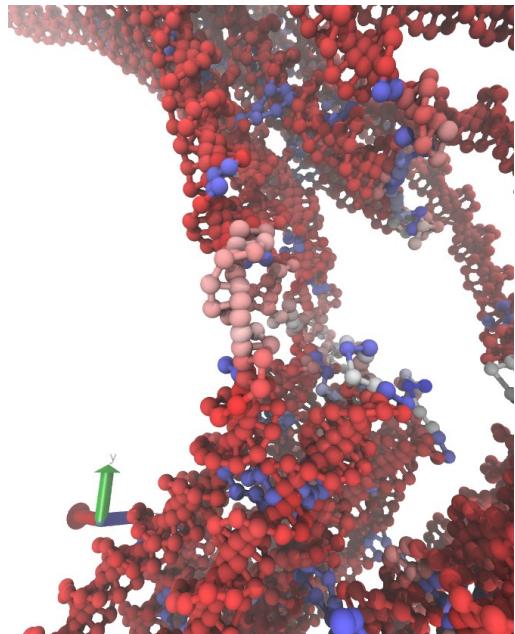
Distribution of
DNA end to end
vector dotted with
direction of applied
force.



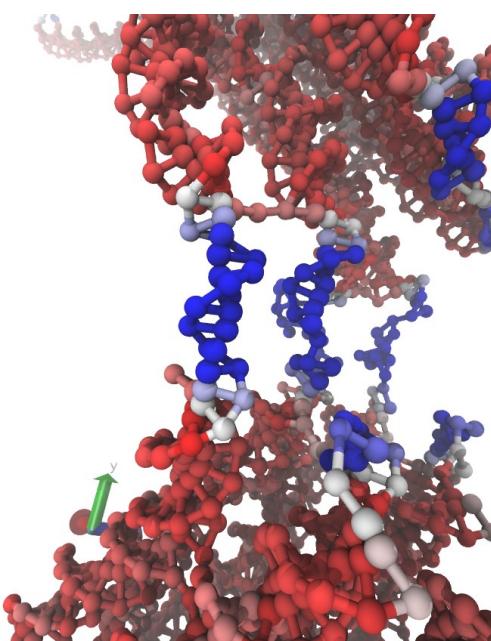
Cross stacking at ssDNA-dsDNA interface stabilizes ssDNA helix.



Hydrogen bonding

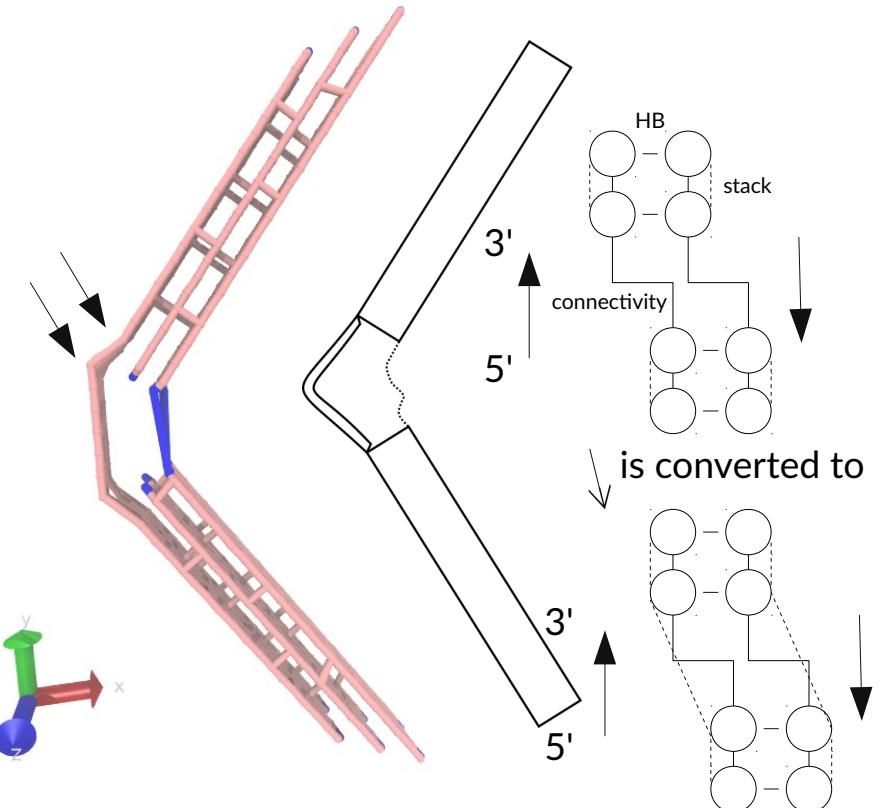


Stacking



Cross stacking.

MrDNA stacking problem



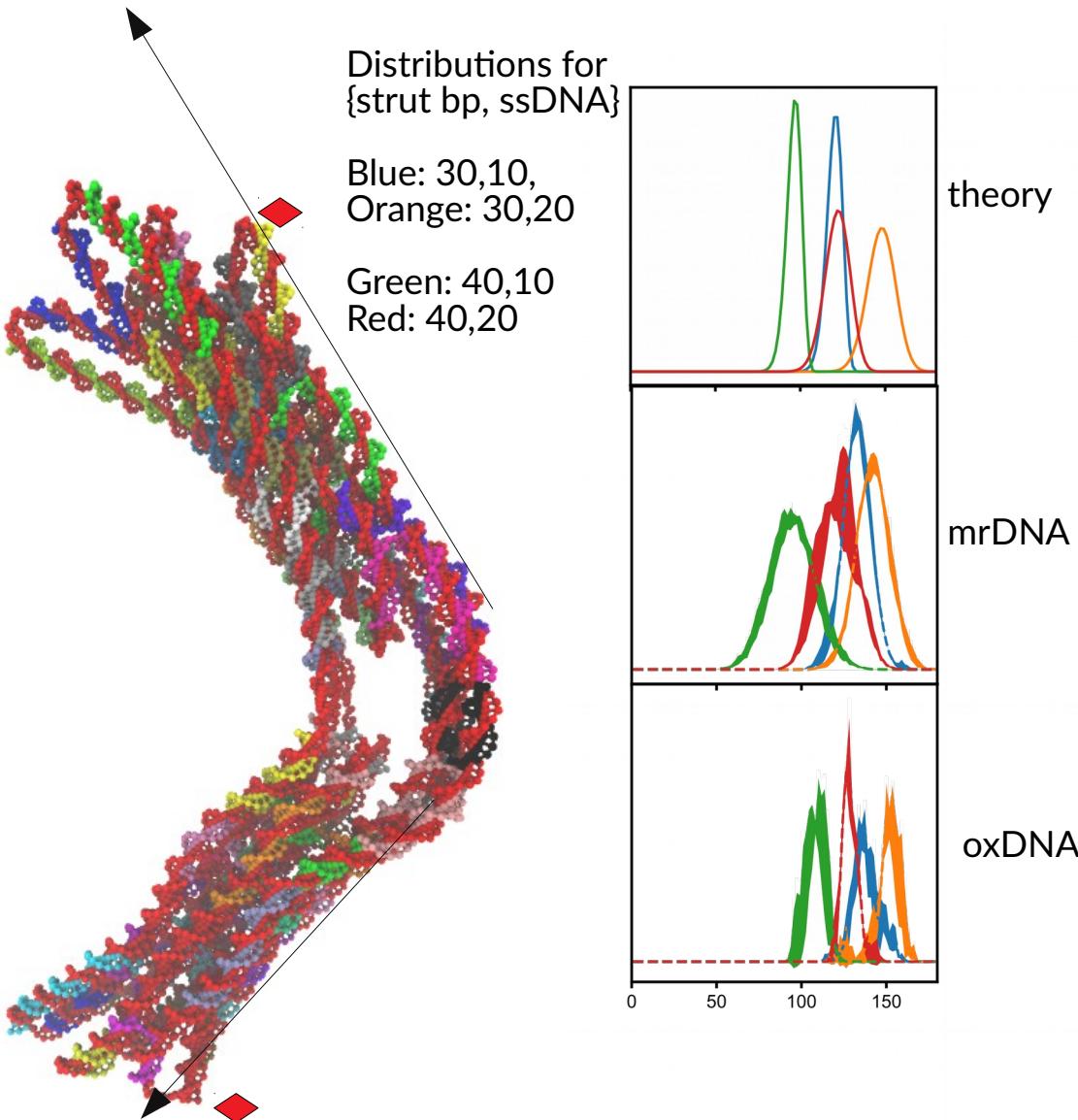
MrDNA is cool but violates some very basic assumptions about how simulation force fields should behave.

Because mrDNA allows co-existence of multiple resolutions simultaneously, the same structure can be described in lots of different ways. 4 ssDNA can be described as:

(2) (2) or (1) (3) etc.

More problematically, the force field depends strongly on the initial configuration. If two things aren't stacked, then mrDNA doesn't think they're part of a contiguous duplex, even if the ultimate structure is the same. This bug appears in all of my mrDNA work so far.

I have fixed the software bug by requiring "if the 3' nt of a bp of a bp's 3' nt is its bp, then all 3' relations here are also stacking relations." Easier to see with diagram. But this means all my mrDNA simulations suck a bit, but oxDNA simulation (probably) not affected. Maybe (but not necessarily) also a problem in MagicDNA -> mrDNA export).



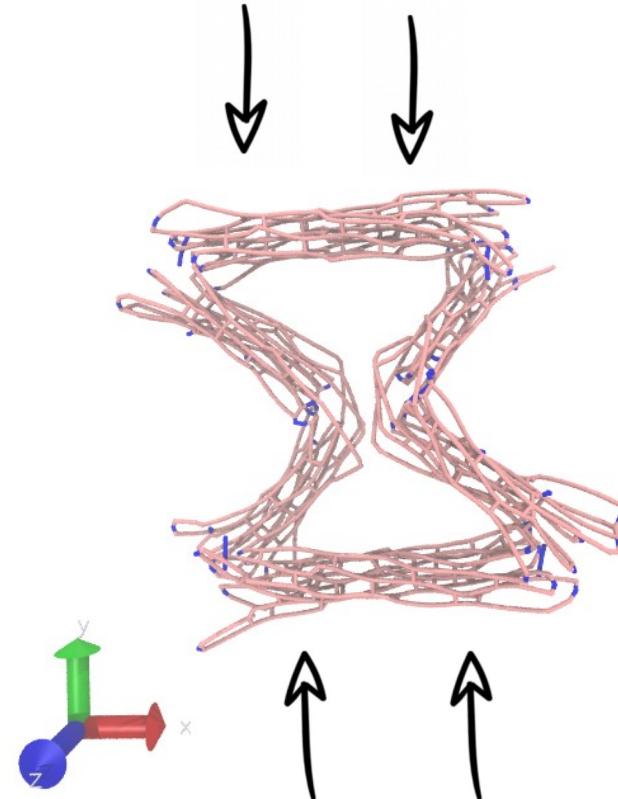
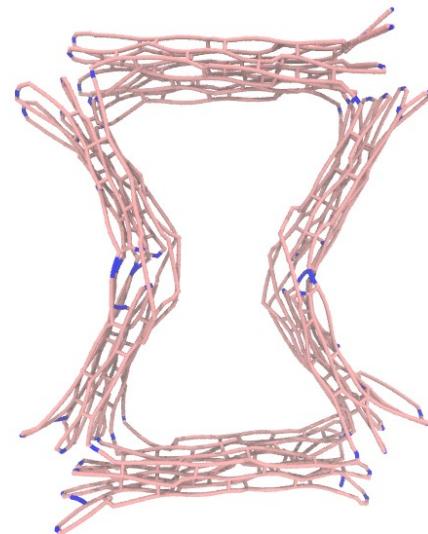
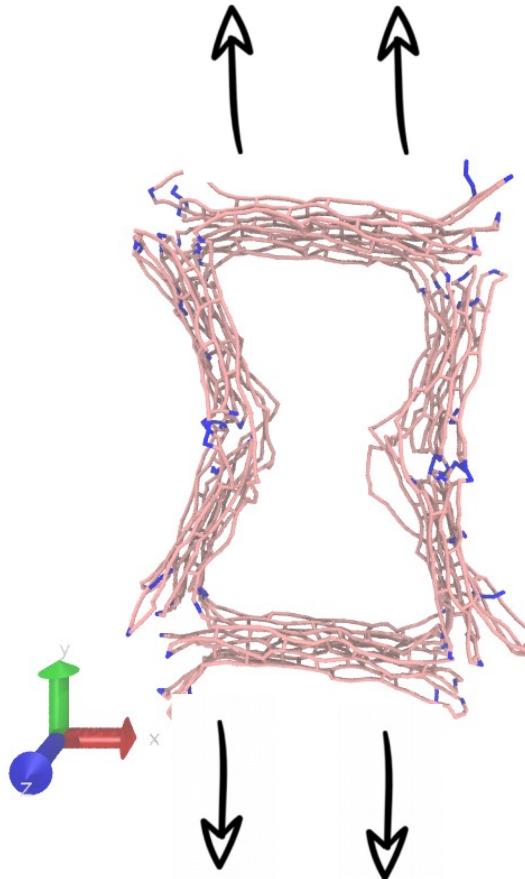
Bending angle distributions

We measure the bending angle in both oxDNA and mrDNA simulations by creating a vector that points along the spine. Vector begins at the central junction, where the bending strut joins the 4x3 cross section beam. Vector ends at the 3 loop scaffold ssDNA that is used to attach other mechanical linkages.

Angle acquired from inverse cosine of dot product of two vectors.

Not that this is a bit sketchy as there's a tendency in mrDNA for dsDNA near the junction to "bow out"

How does the entire structure deform under compression / expansion?



(Haven't figured out quantitative details for analysis but have run simulations... just need to analyze.)

Next steps

Experimental

Buy staples for structure with increased number of ssDNA at hinge joint.

Anneal each of the mechanical linkages on its own, and AFM / TEM.

Anneal the mechanical linkages together, and AFM / TEM.

(In principle you could have genuine modular design, where you have 5 different compliant joints, and 5 different hinges, then design for interface so you could make 25 structures... not impossible...)

Numerical

Finish mechanical compression / expansion, to estimate stiffness directly from simulation.

Polish up some of the theory stuff.