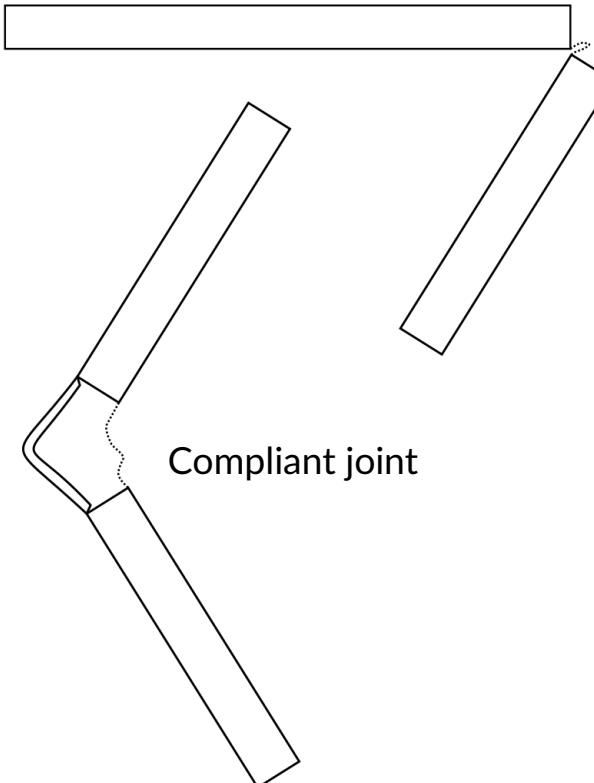
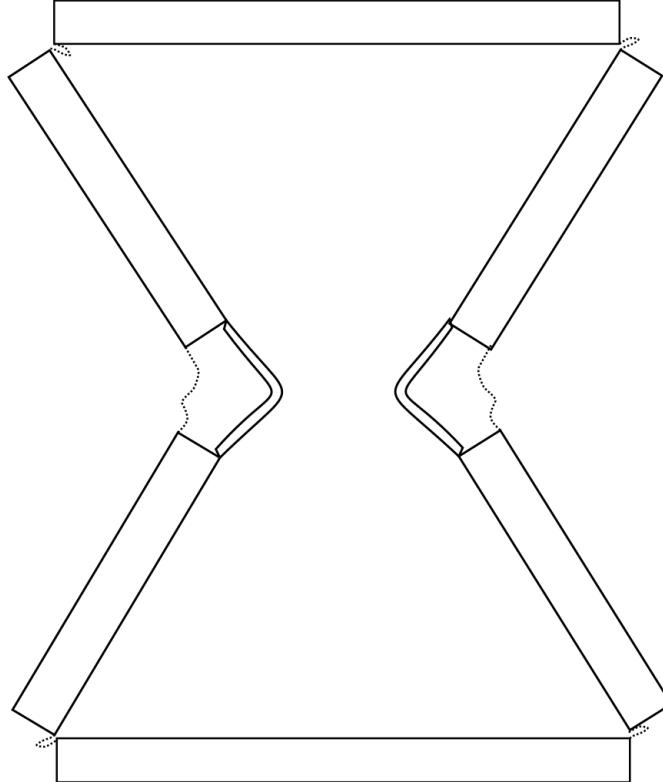


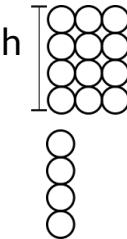
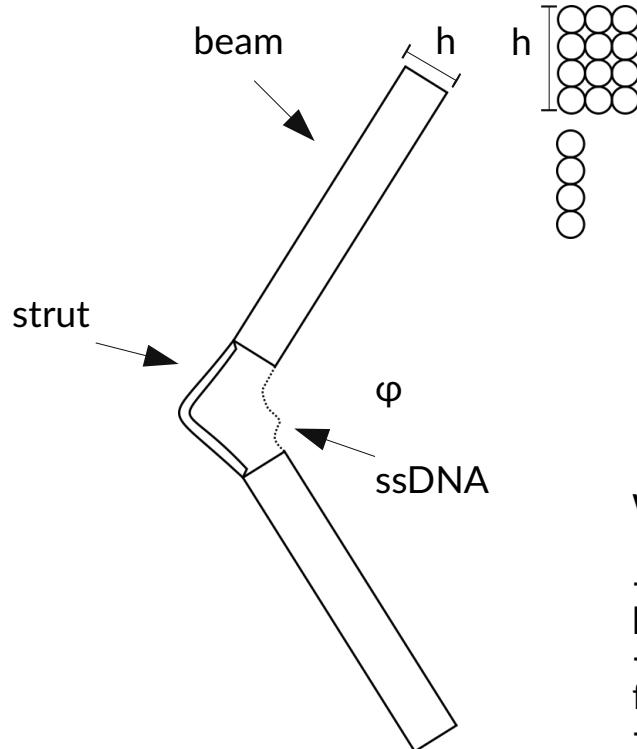
# Honeycomb monomer



Hinge

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

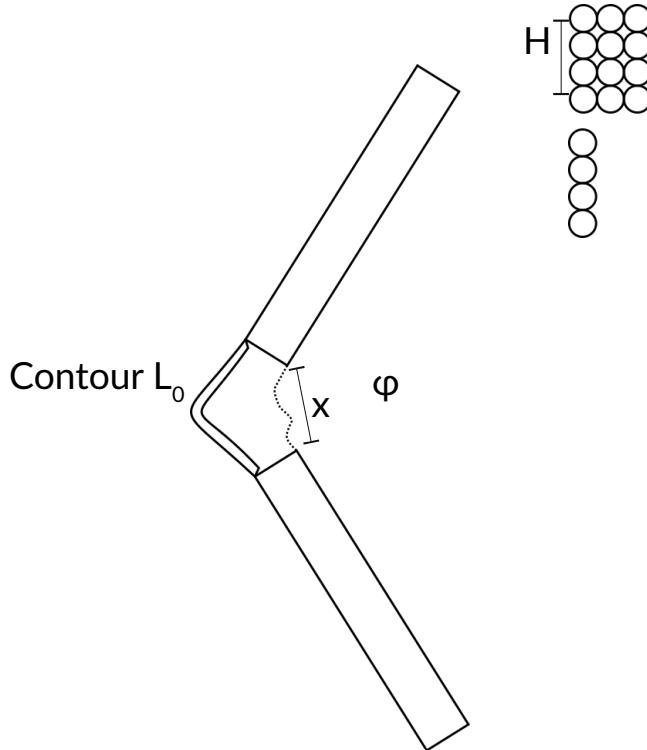
Department of Mechanical and Aerospace Engineering

The Ohio State University

Columbus, Ohio, USA

Email: zhou.809, marras.3, castro.39, [su.298@osu.edu](mailto: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

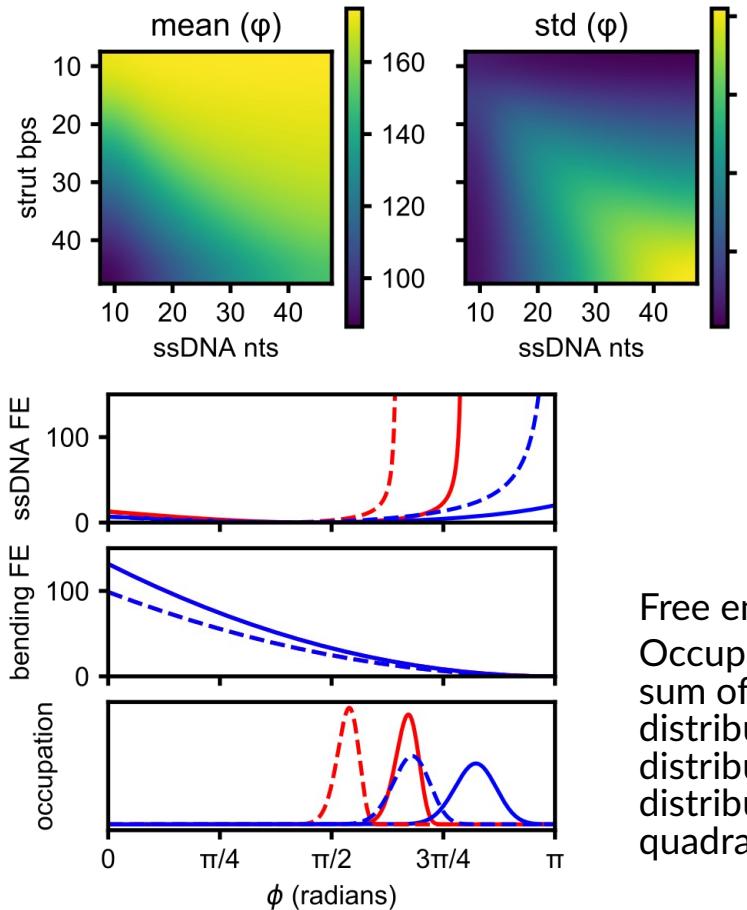
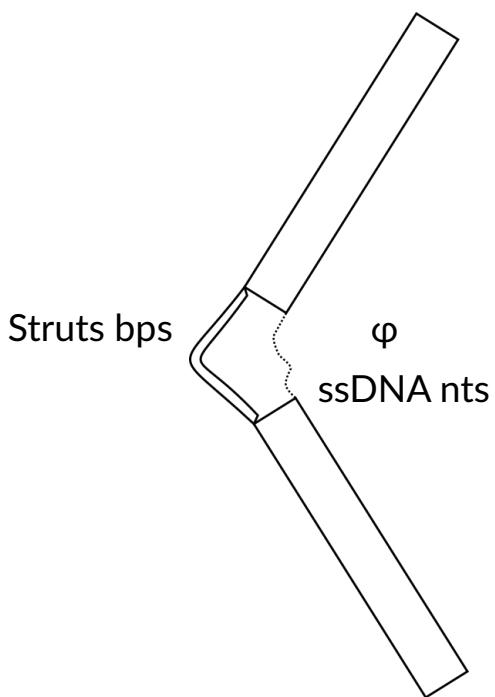
→ Treat as power expansion of WLC

→ 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.

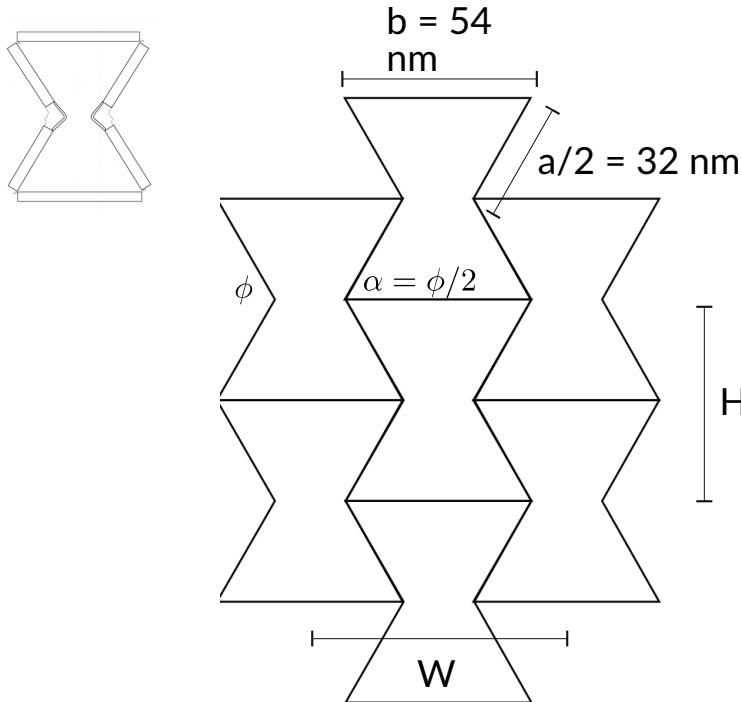
Unexpected: Angle distribution width is re-entrant in both number of strut base pairs, and in number of single stranded nucleotides.

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 quadratic potential.

## Constitutive relationship of a material with unconventional Poisson's ratio

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E-mail: alan\_tc\_lim@yahoo.com



# 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:

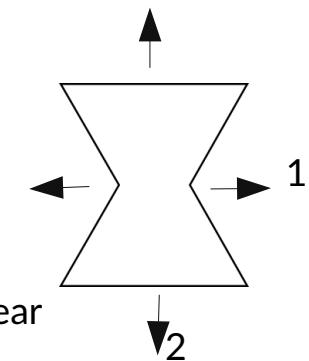
$$\nu_{12} = -\frac{\sin \alpha \tan \alpha}{2b/a - \cos \alpha}$$

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

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

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

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



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

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

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

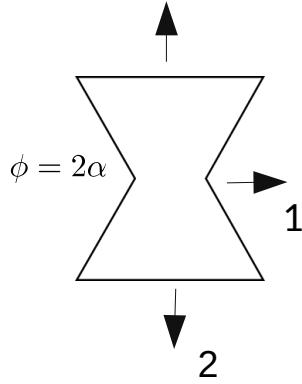
How hard to widen?

How hard to lengthen?

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

How hard to shear?

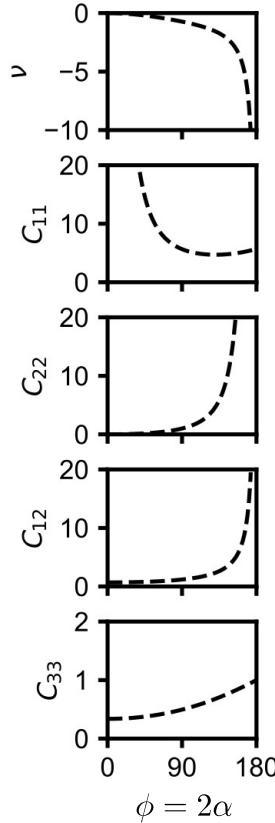
# Analytical treatment of honeycomb



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

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

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



(-) 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?

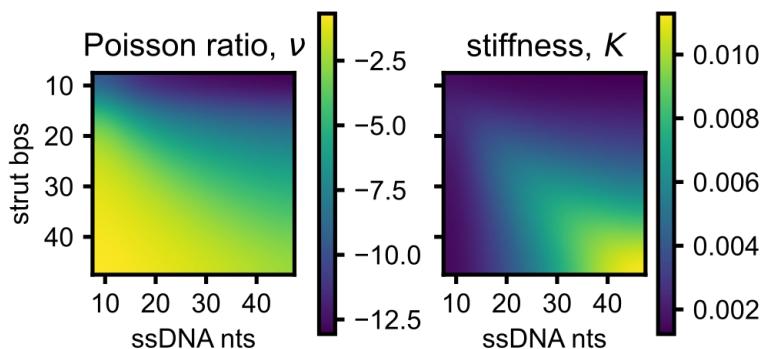
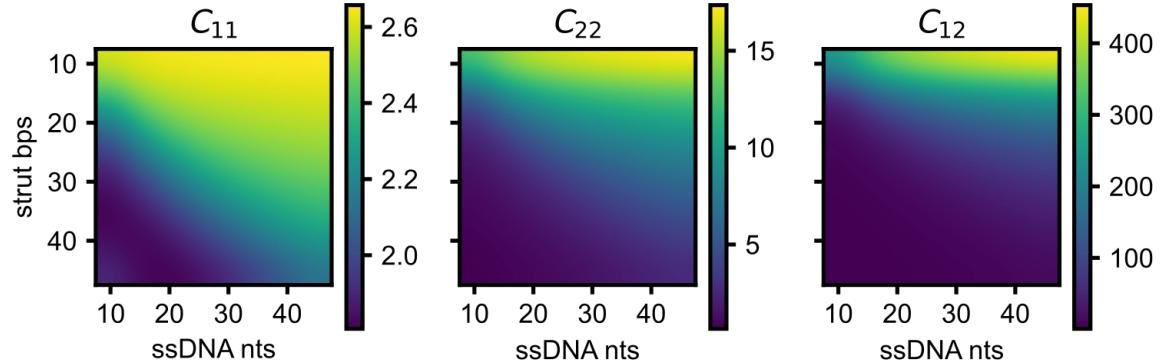
Various physical quantities diverge, including the Poisson ratio.

$C_{22}$  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 ( $\phi \rightarrow 180$ ).

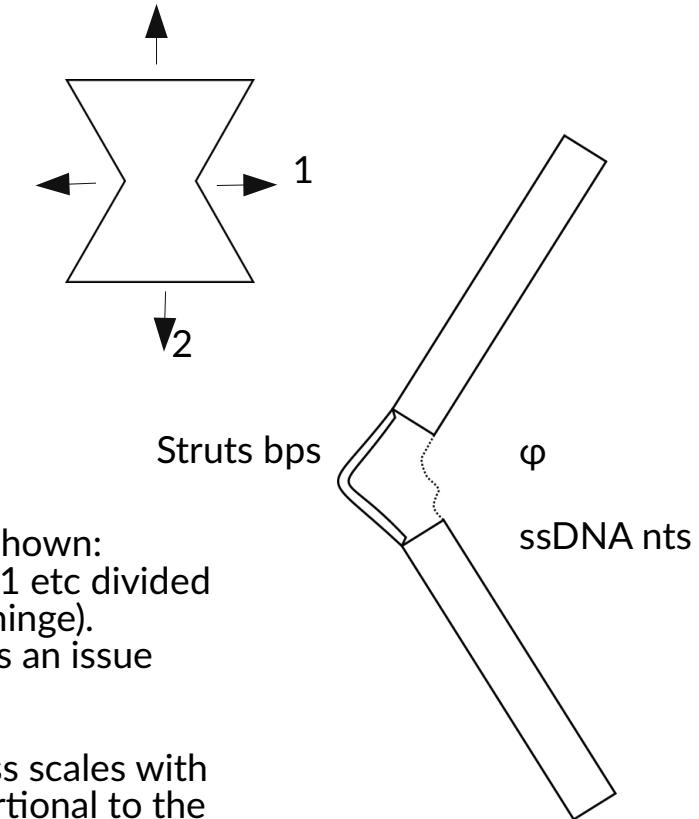
$v_{12}$  as described here is the ratio of horizontal strain to vertical strain. At  $\phi = 180$ , the derivative of height wrt  $\phi$  is 0, but the derivative of width wrt  $\phi$  is not 0. Therefore  $v_{12}$  diverges (while  $v_{21}$  is 0 here, as the two Poisson ratios are inverses).

# What would the parameters of our material be?

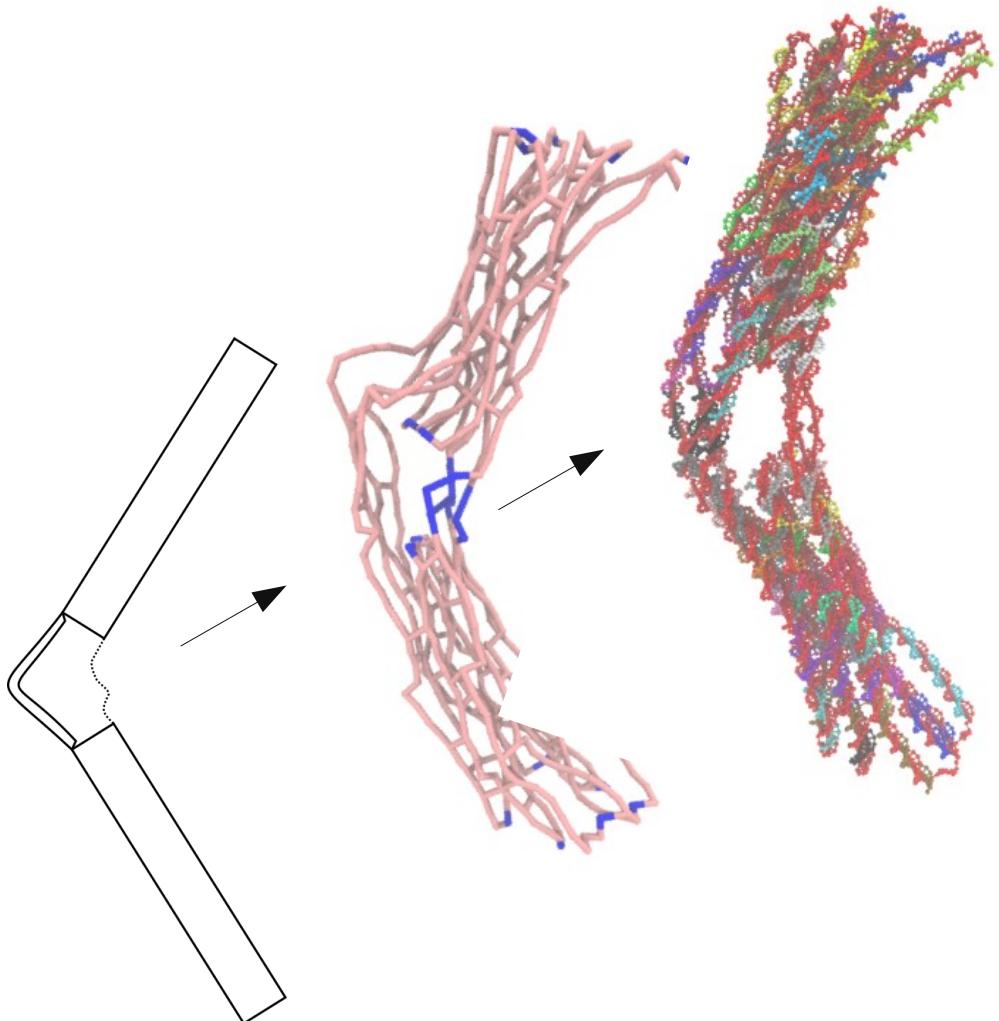


Various geometrical stiffnesses shown:  
(geometrical stiffness  $\rightarrow$  True C<sub>11</sub> etc divided by  $K$ , which is a property of the hinge).  
Haven't put units because there's an issue with volume...

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...



# 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.

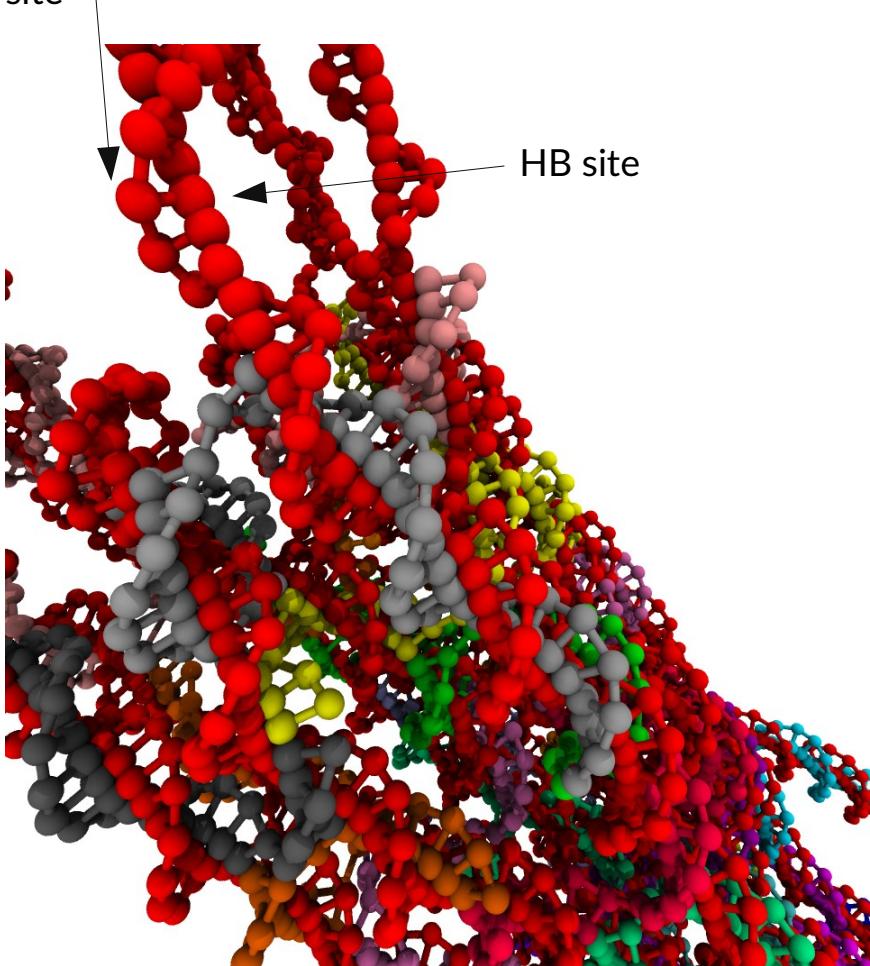
I wrote an oxDNA -> mrDNA converter which generates mrDNA structures from oxDNA structures (this wasn't trivial... I needed to use some clever datastructures to make this time and space efficient. I'll write it up and put a link to my Github on the oxDNA slack).

I then simulate in mrDNA (using a GPU) for about  $1 \times 10^7$  timesteps using 5 bp per bead, then for an additional  $1 \times 10^7$  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 (72 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.

Don't want to release it to the oxDNA community because it kind of undermines what the oxdna-viewer Javascript guy has been doing.

WillTKaufhold1/will\_oxdr 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](https://github.com/WillTKaufhold1/will_oxdna_vmd)

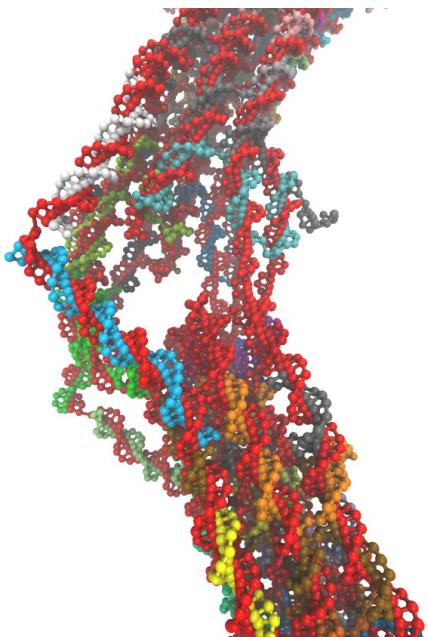
But not actually sure if I want to release it because it might annoy oxdna-viewer guy.

My system is much much better than anyone else's though :)

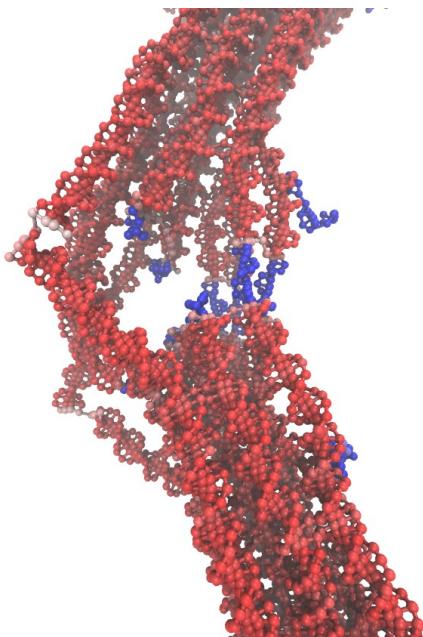
Reason mine is better than all of others:

Explicit visualization of energy distribution.

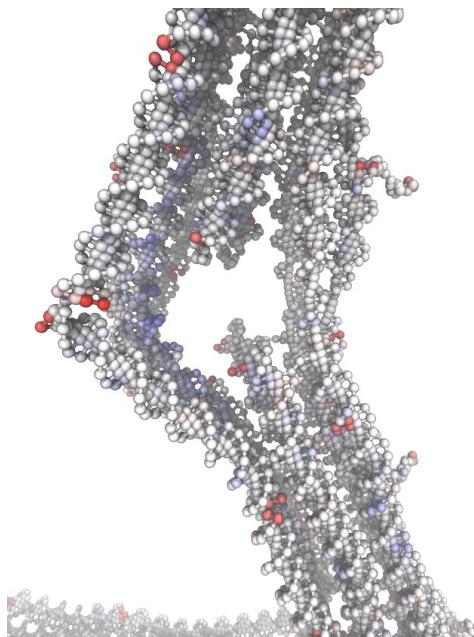
# Seeing $\langle$ energy $\rangle$ is great for insight.



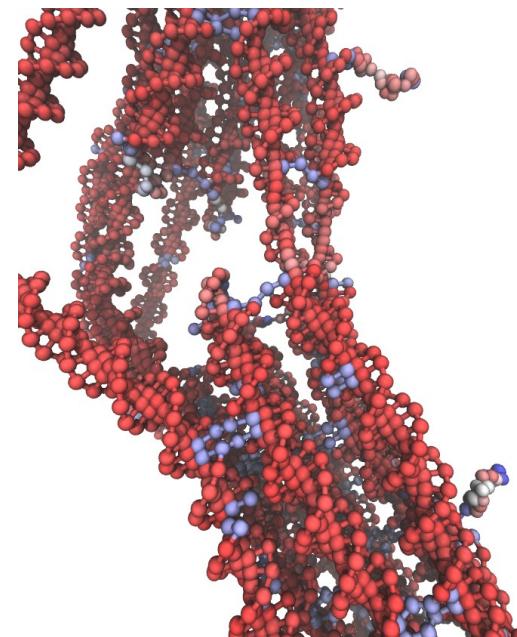
Strand identity



Hydrogen bonding



Backbone stretching



Stacking



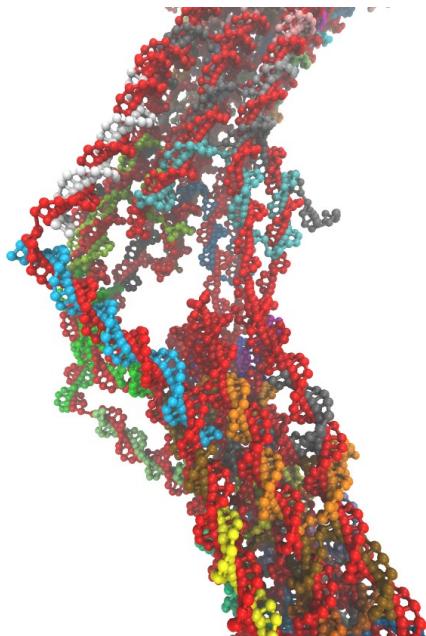
Favorable



Unfavorable



# Have a look at these features



Strand identity

Hydrogen bonding

Backbone stretching

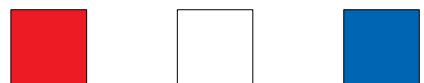
Stacking

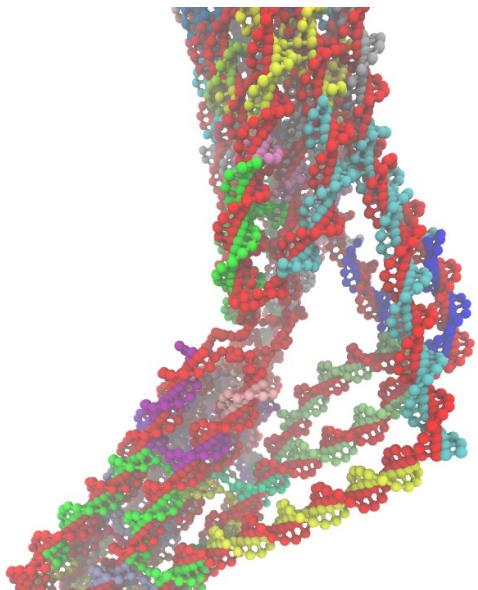
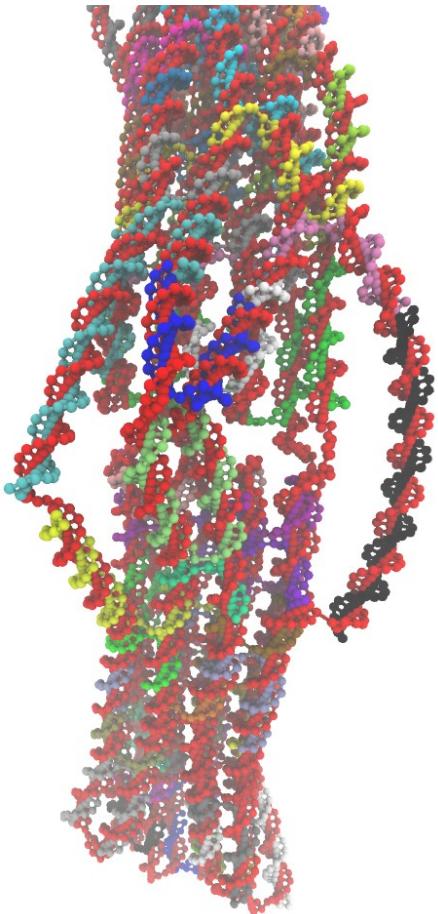


Favorable



Unfavorable





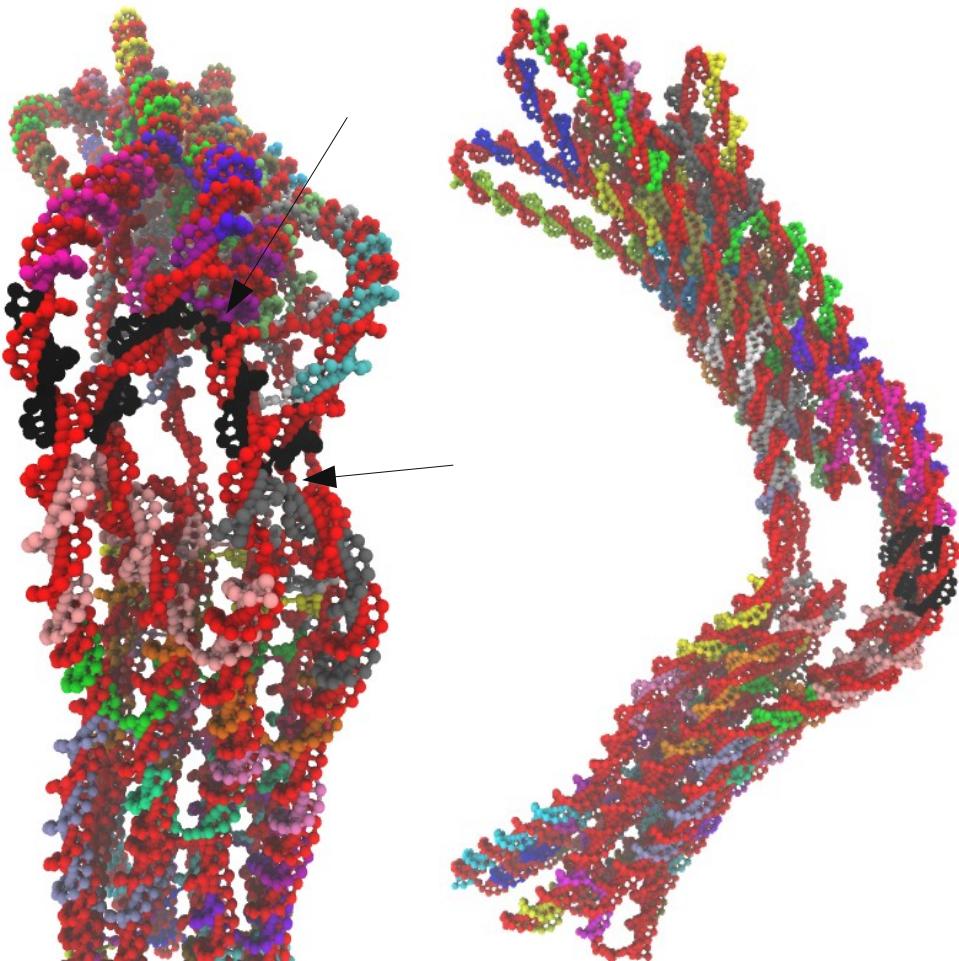
# strut = 30 buckles

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.

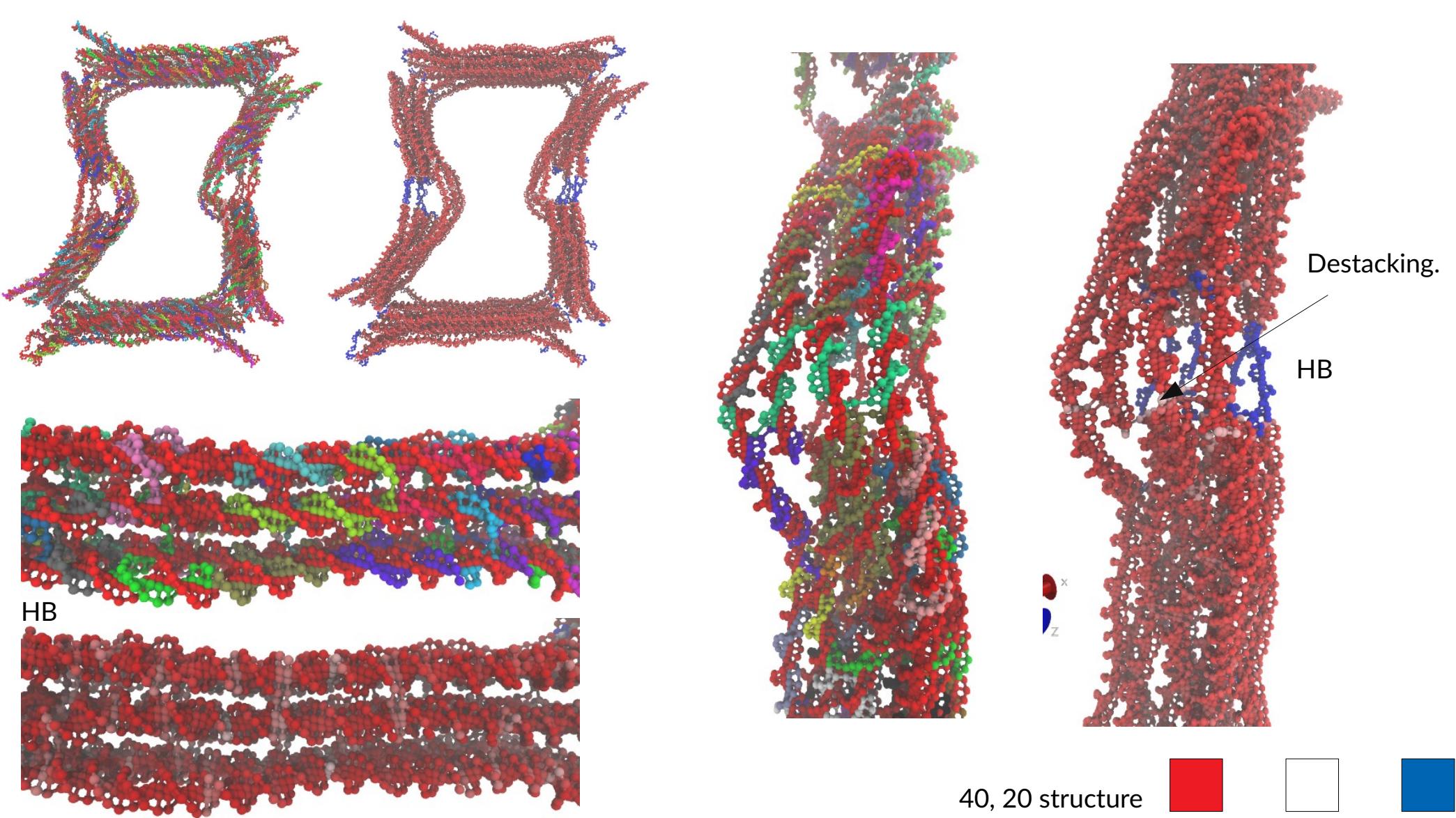
strut = 40 bends rather than buckling.

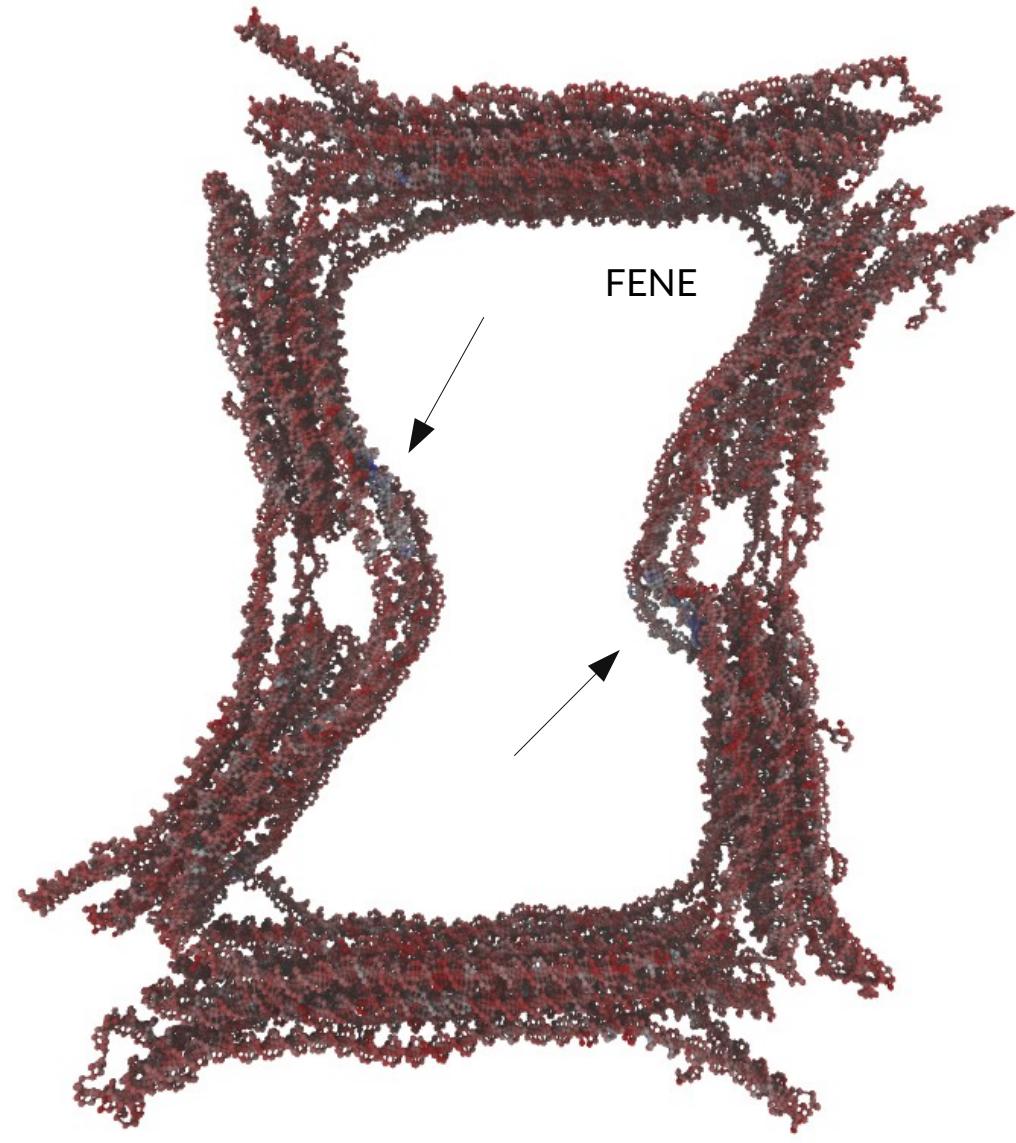


For the  $4 \times 1$  strut, there are two outside crossovers (i.e. between the left two and the right two helices), and two inside crossovers (i.e. just between the two inner crossovers).

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

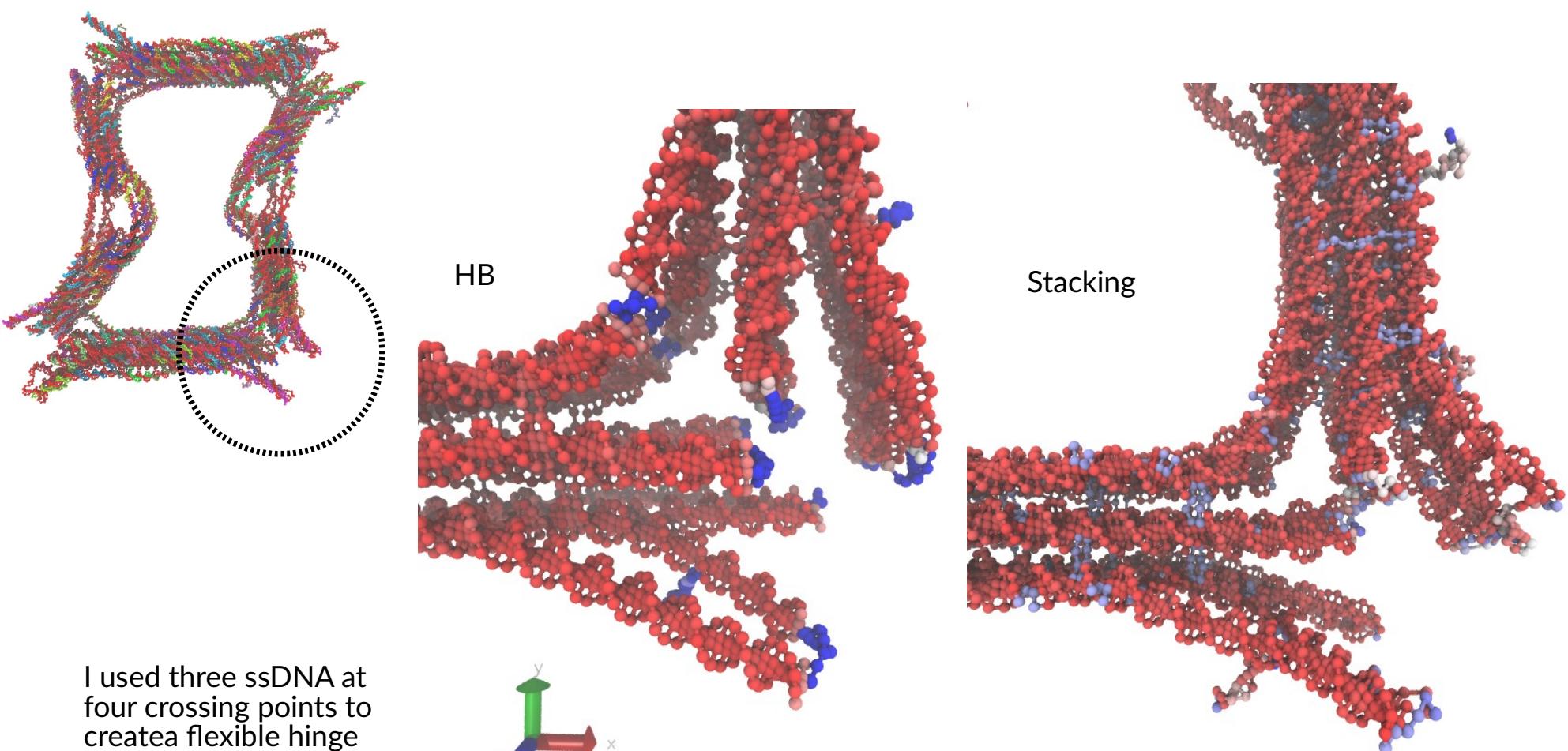
Would be very easy to do a systematic study of how crossover distribution affects buckling. (but let's not get even more distracted)



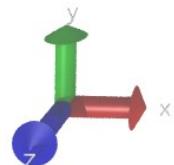


FENE energy distribution over compliant strut very lopsided... our analytical model of the hinge predicts a symmetric distribution... so does basic intuition...

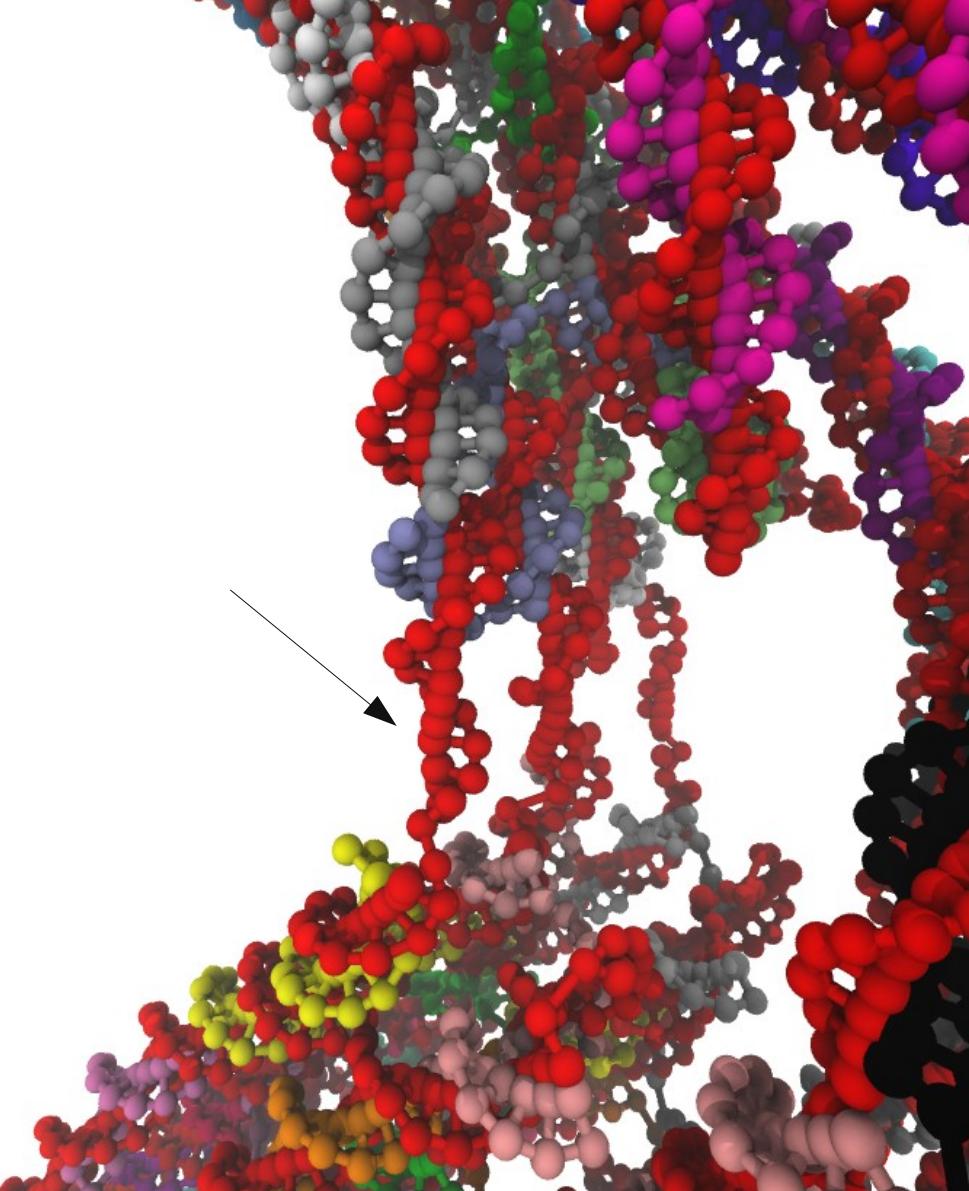
Notice also the entire hourglass is sheared a bit... non uniform FENE distribution over compliant joints probably linked to shear.



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.



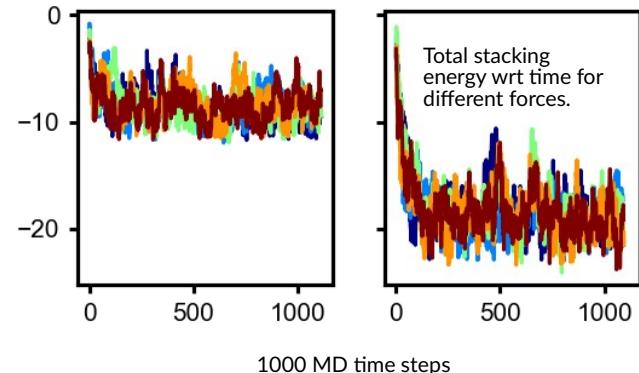
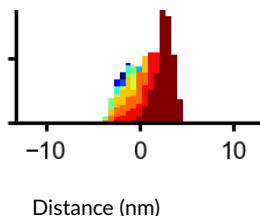
# ssDNA in bridge is helical.



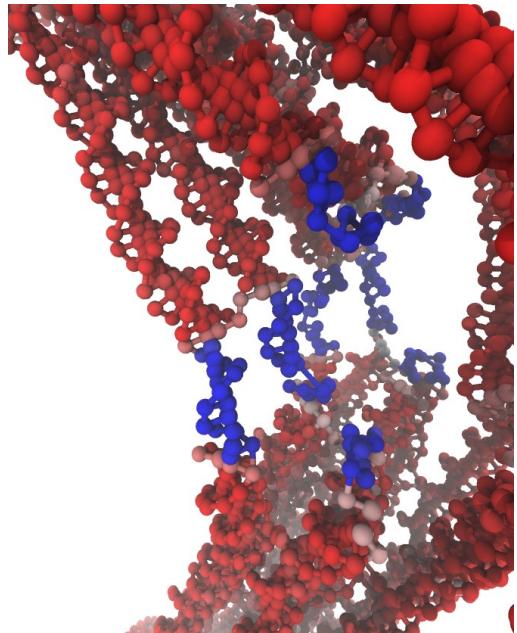
Is it obvious that single stranded DNA under tension becomes helical? I would have thought this should happen... if you tension a single strand of DNA, then you increase the energy of configurations which aren't colinear with the applied force.

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?

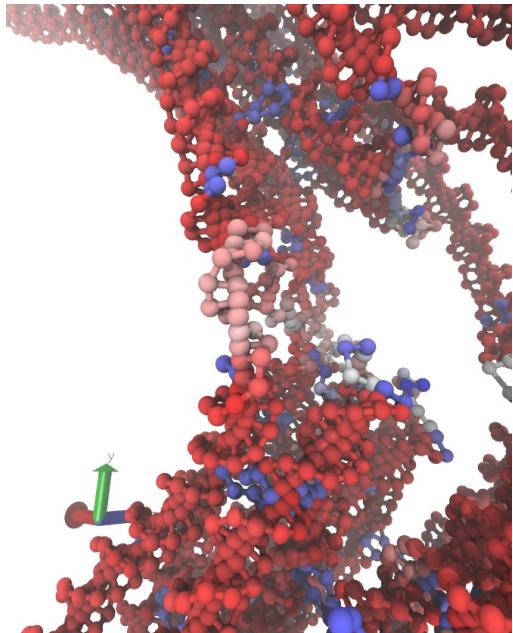
Distribution of  
DNA end to end  
vector dotted with  
direction of applied  
force.



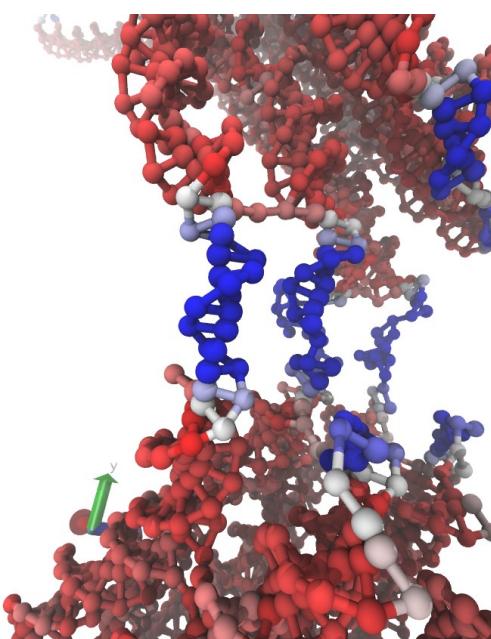
# Cross stacking at ssDNA-dsDNA interface stabilizes ssDNA helix.



Hydrogen bonding

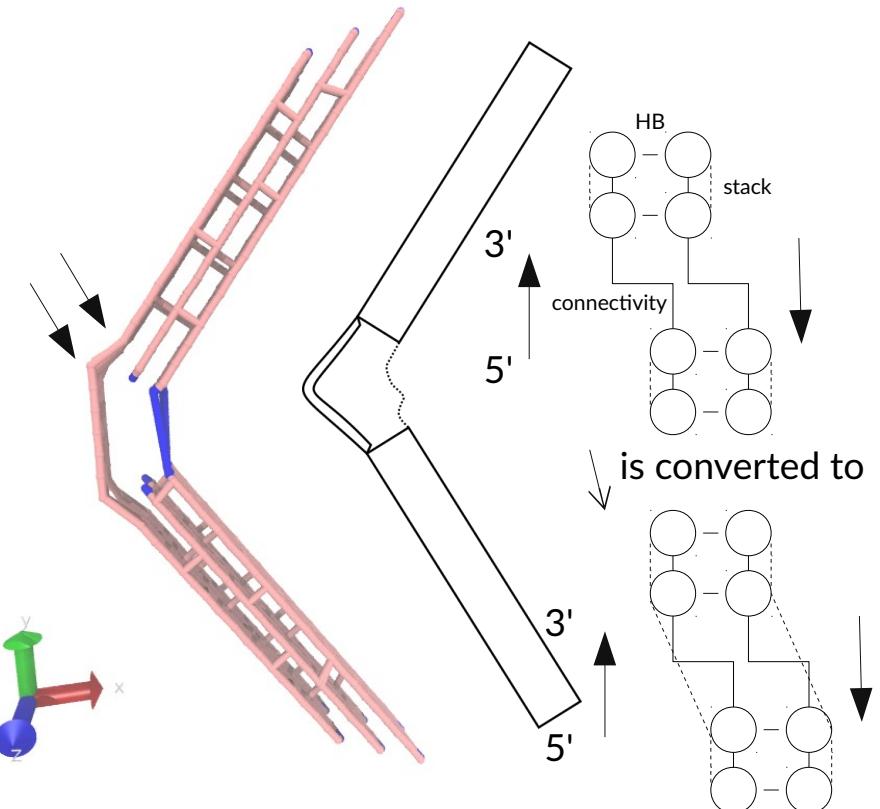


Stacking



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:

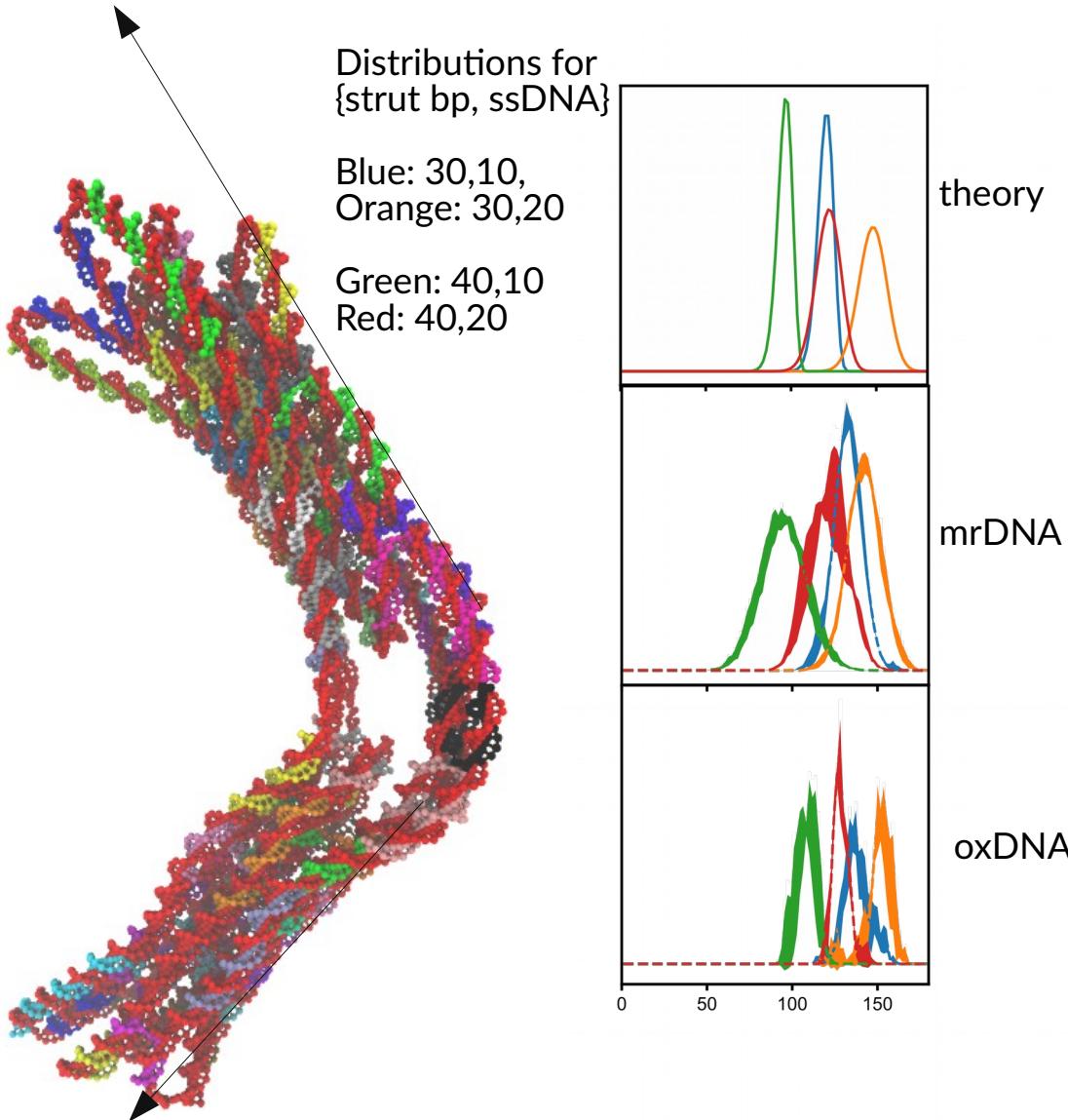
(2) (2) or (1) (3) etc.

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 mrDNA simulations suck a bit, but oxDNA simulation (probably) not affected.

Might also try fixing the mrDNA magicDNA export fix if magicDNA is also broken there.

# Bending angle distributions

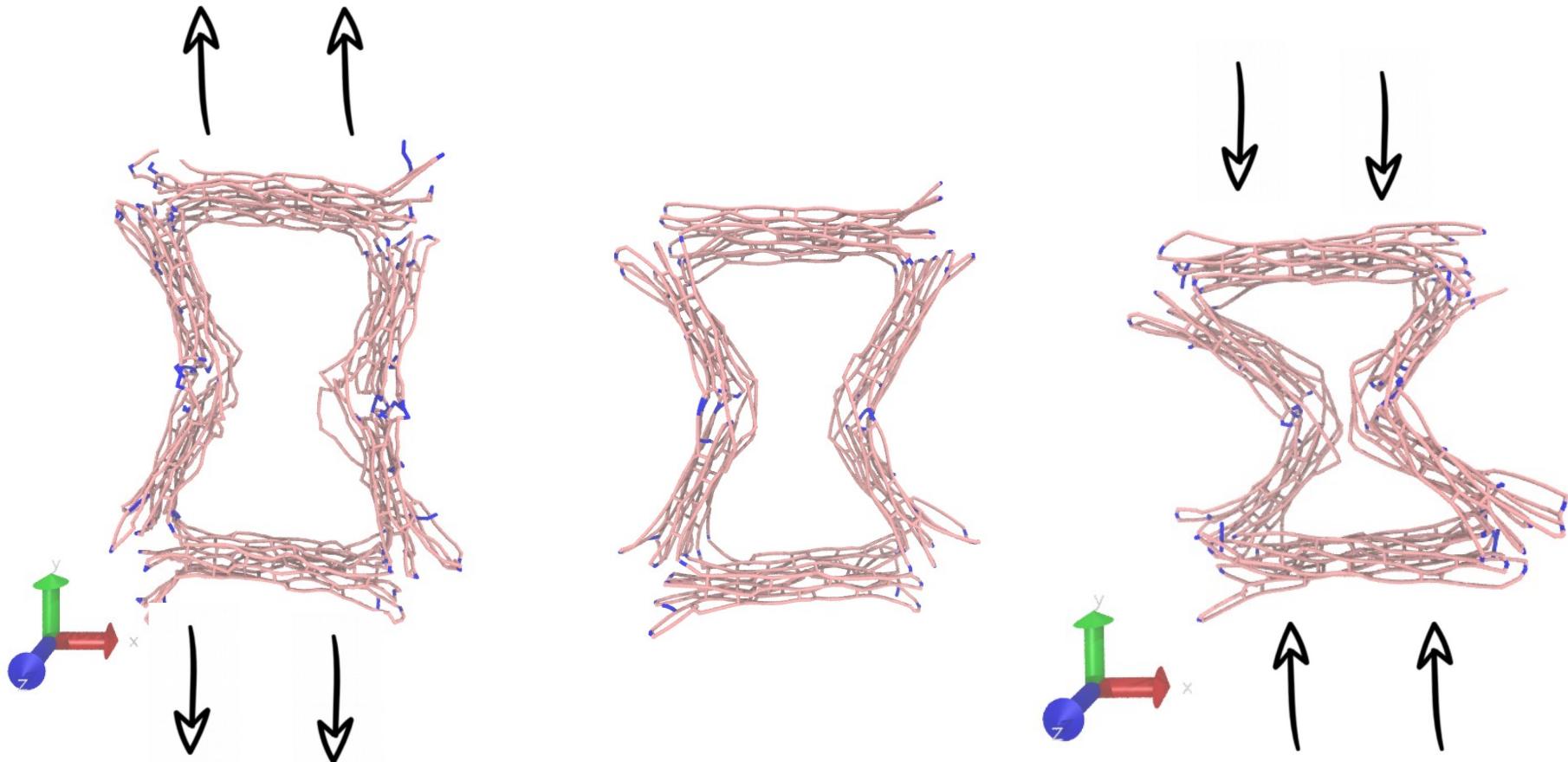


We measure the bending angle in both oxDNA and mrDNA simulations by creating a vector that points along the spine. Vector begins at the central junction, where the bending strut joins the 4x3 cross section beam. Vector ends at the 3 loop scaffold ssDNA that is used to attach other mechanical linkages.

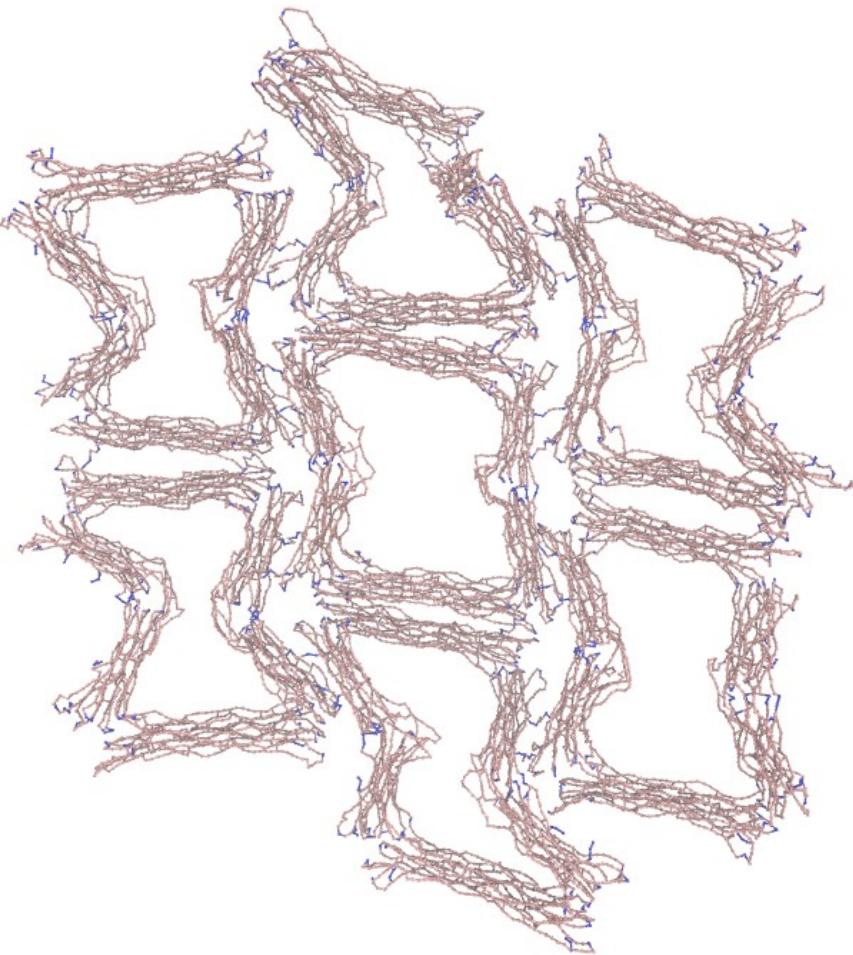
Angle acquired from inverse cosine of dot product of two vectors.

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?



# Structures tessellate



(And if we want we can simulate material patches using mrDNA, possibly with additional forces)

# 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)

## Numerical

Finish mechanical compression / expansion, to estimate stiffness directly from simulation.  
Polish up some of the theory stuff.  
I think this basically fine? Could always do entire material patch simulation, but seems a bit vain...