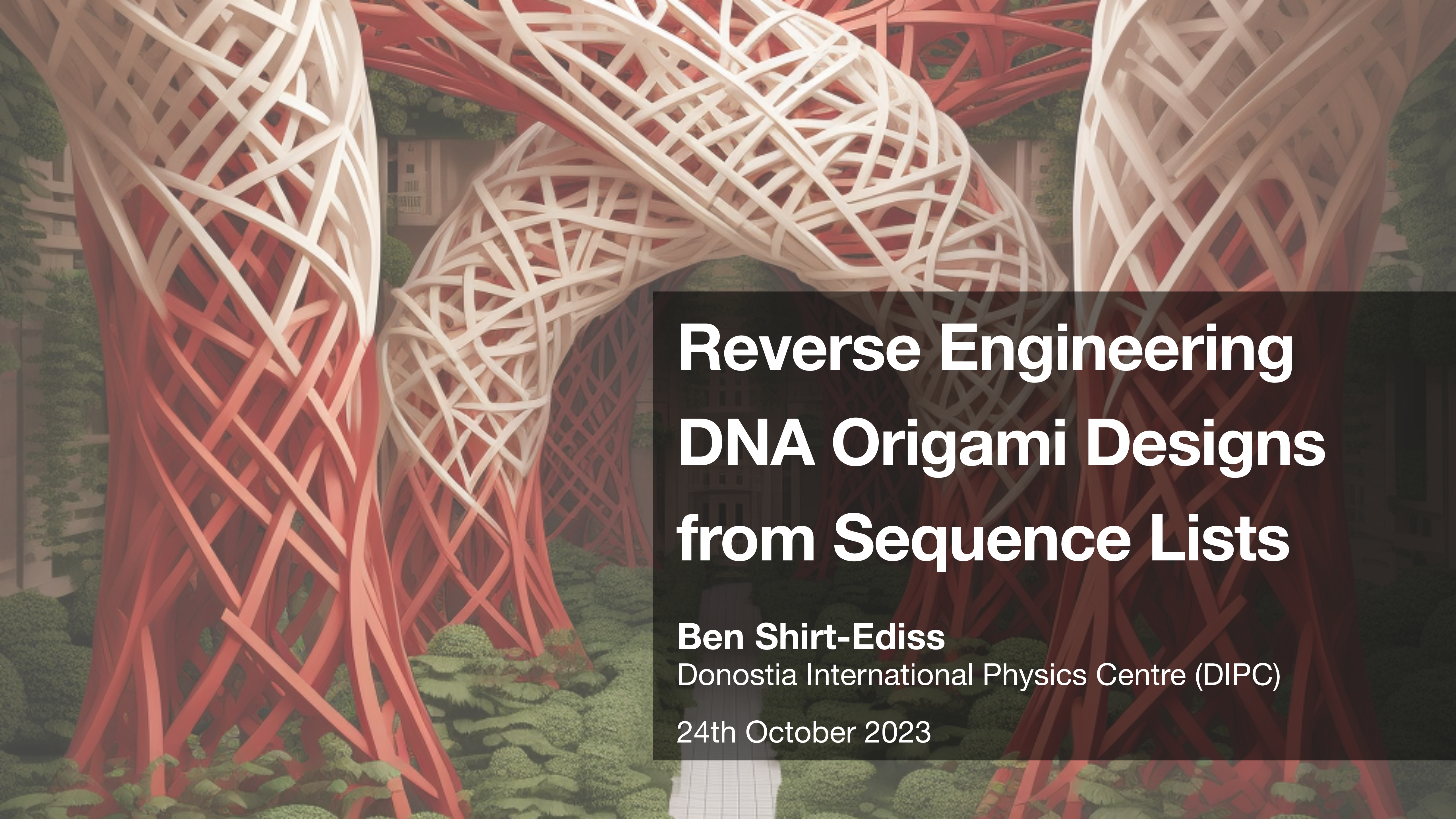




Reverse Engineering DNA Origami Designs from Sequence Lists

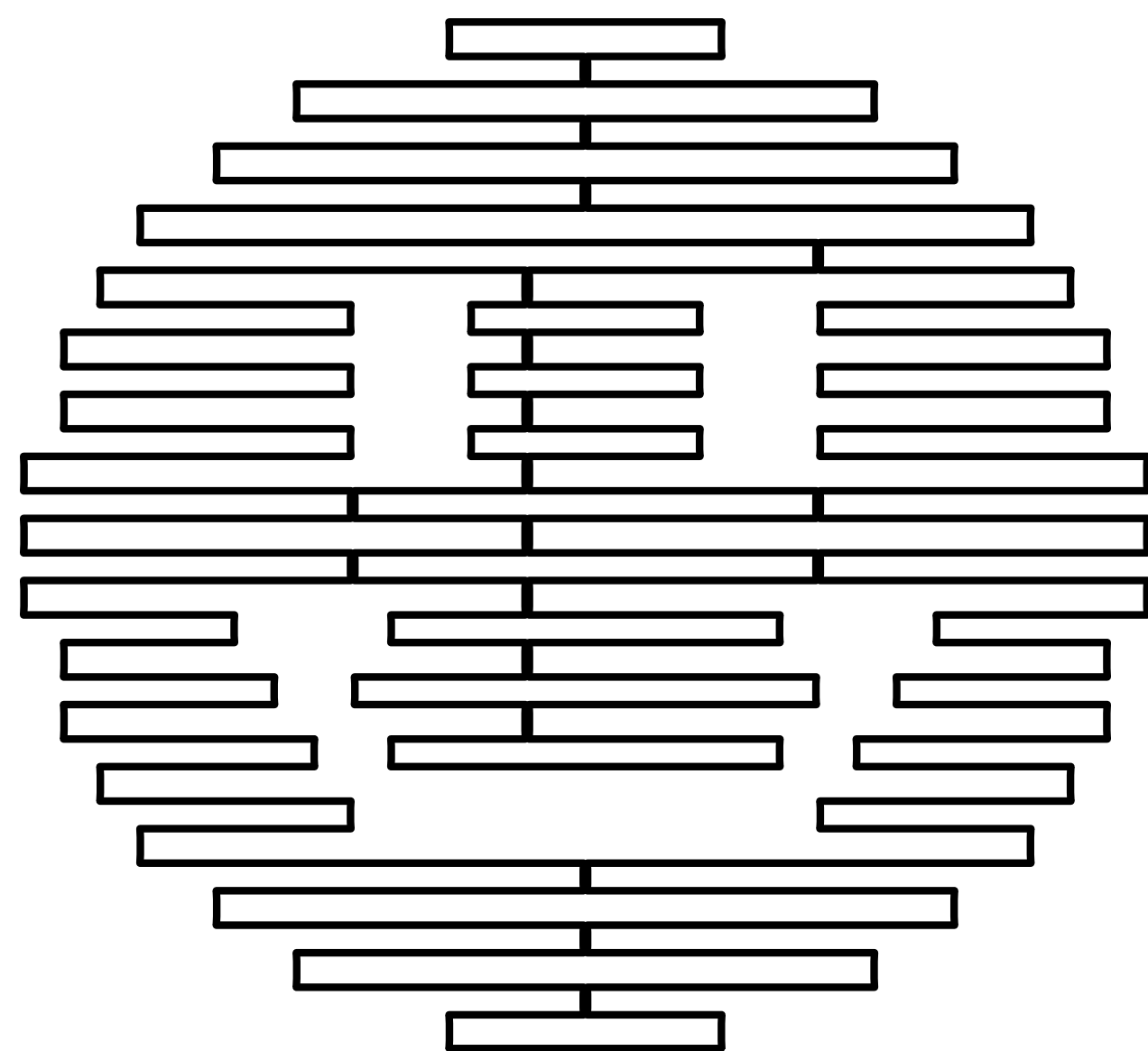
Ben Shirt-Ediss

Donostia International Physics Centre (DIPC)

24th October 2023

Traditional DNA Origami Design

Design File



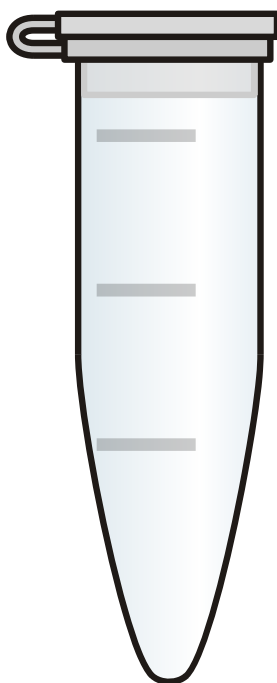
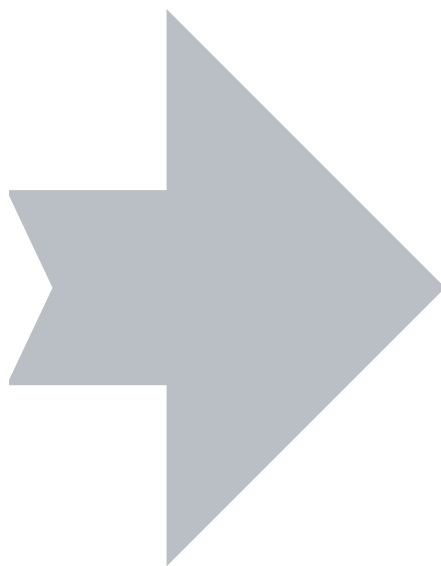
Raw Published Sequences

Scaffold

```
CTCACTGATTATAAAAACTTCTCAGGATTCTGGCGTACC
GTTCCCTGTCTAAAATCCCTTTAATCGGCCTCCTGTTTAGCT
CCCGCTCTGATTCTAACGAGGAAAGCACGTTATACGTGCT
CGTCAAAGCAACCATAGTACGCGCCCTGTAGCGGCGCATT
AAGCGCGGCGGGTGTGGTGGTTACGCGCAGCGTGACCG
CTACACTTGCCAGCGCCCTAGCGCCCGCTCCTTTCGCTTT
CTTCCCTTCTTTCTCGCCACGTTGCGCCGCTTTCCCCGT
CAAGCTCTAAATCGGGGGCTCCCTTTAGGGTTCCGATTTA
GTGCTTTACGGCACCTCGACCCCAAAAACTTGATTTGGG
TGATGGTTCACGTAGTGGGCCATCGCCCTGATAGACGGTT
TTTCGCCCTTTGACGTTGGAGTCCACGTTCTTTAATAGTGG
ACTCTTGTTCCAAACTGGAACAACACTCAACCCTATCTCGG
GCTATTCTTTTGATTATAAGGGATTTTGCCGATTTGGAAC
CACCATCAACAGGATTTTCGCCTGCTGGGGCAAACCAGC
GTGGACCGCTTGCTGCAACTCTCTCAGGGCCAGGCGGTG
AAGGGCAATCAGCTGTTGCCCGTCTCACTGGTGAAAAGAA
AAACCACCCTGGCGCCCAATACGCAAACCGCCTCTCCCC
GCGCGTTGGCCGATTCAATAAT. . .
```

Staples

```
CCGTTGAATTAA
GTCTGTCCATCAGCATAGCAATACTTCTTTGAACTCAAA
AGTAGAAGATTAGTAATAACATCAATCGGAAC
CCTAAAGGTGCCGTAAAGCACTAACTTGCCTG
CGAGAAAGGAAGGGAAGCCACCGAGTAAAAGA
CTATCGGCTGGATTATTTACATTGAGGGACAT
AGAACCCTGCTCAATCGTCTGAACTTGCTGGTAATATCC
AGAACAATATTACCGCATACCTACATTTTGACTCTGACCT
GTGGCACAAAAACGCTCATGGAACAGCCATTGCAACAGG
CAAATATCTAGCCCTAAAACATCGAAGAATAC
GAAAGCGTCCATTAAAAATACCGACTAAAGCATCACCTTG
TAGTCTGGCTAT
GACAATATTTTTGAATTTAATGCGCGAACTGAAAACCTC
GTAATAAAGCAGATTCACCAGTCAATAGGGTT
.
.
.
```



Physical
Self-Assembly

High Quality Design Schematics: Often Not Published

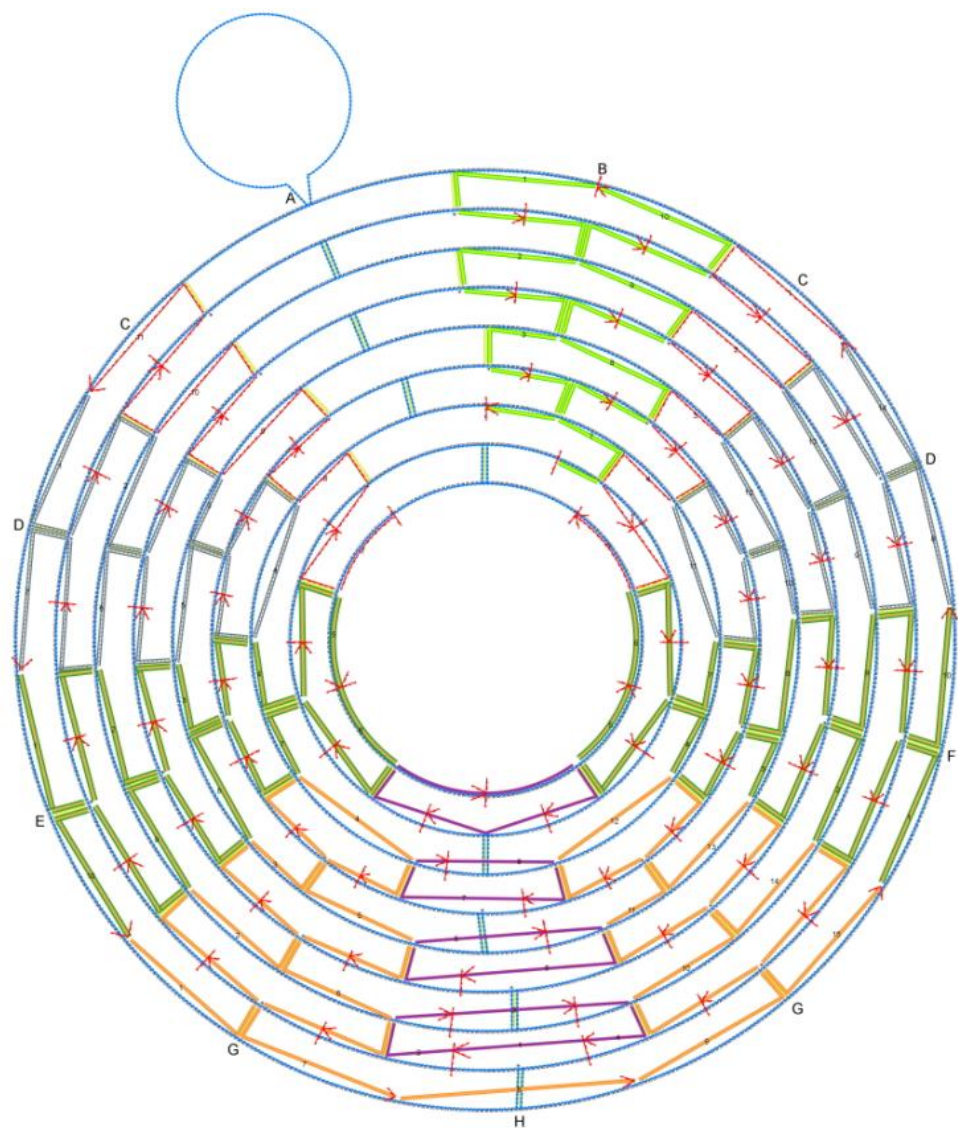


Figure S27. Schematic diagram of the ‘opened’ 9-layer concentric ring structure. The open structure is the same as the 9-layer concentric ring structure shown in Figure S26, with several staple strands removed. In region A, staple strands 1-8 are not included. In region B, staple strands 5 and 6 are not included. In region C, staple strand 6 was not included. The exclusion of these staple strands, which are intended to traverse all 5 scaffold crossovers on one side of the structure, effectively removes the link between regions B and C. The result is an open, concentric ring structure. All applicable staple sequences are the same as for the unmodified 9-layer ring structure.

Table S11. Sequences of the staples in the 9-layer concentric ring structures.

Region A	
A1	AATAGTAGTAGCATTGCGCCTGTTTATCAA
A2	CAATAGATAAGTCCTAAAAACAGGGAAGC
A3	GCATTAGACGGGAGTAACCCCTCGTTTAC
A4	CAGACGACGATAAAGGCATCAATTCTACT
A5	GCAACACTATCAAATTAAGTGAACACCCTGAACAAAGGGGAGGGAAGG
A6	TAAATATTGACGTGTATCATCGCCTGATAAATTGTAGGCATAGTAAGA
A7	ACAACGGAGATTGAAATTATTCATTAAACCCTCAG
A8	AGCCACCACAAATCTCCAAAAAAGCGCGAAACAAAGT
Region B	
B1	ATTTTCATTTGGGGCGCGAGCTGAAAAGGTAACCAAAATAGCGA

B2	GAGGCTTTTGCAAATACATAACGCCAAAAGGAATTACGGTCGAAATCCG
B3	CGACCTGCTCCAGCGATTATACCAAGGCTCCAAAA
B4	GGAGCCTTTGAATTGCGAATAATA
B5	ATTTTTTACGTTGACCTCAGAGCCGCCACCGTATAAACA
B6	GTAAATGCCCCCTGCAGAACCGCCACCCTC
B7	AGAGCCACCAAAGGAACAATAAAGAATTGTATC
B8	GGTTTATCAACTAAACACTCATCTTTGACCCCCATGTTACTTAG
B9	CCGGAACGAGGGGAATACCACATTCAACTAATGCAGAAGAAGTTTTGCC
B10	AGAGGGGGTAATAGTCGCAATGGTCAATAACCTGTTTAGCTAT
Region C	
C1	AGTAGATTTAGTTTGACCATTAGATACATTTAAAATGTTTAGAC
C2	TGGATAGCGTCCAAAGAAAGATTGATCAGTTGAGATTTACGCAGACGGTC
C3	AATCATAAGGGGAGAGGCAAAAGAATACGCTTGCTT
C4	TCGAGGTGACGGAGTGAGAATAGACCCTCATTTTCA
C5	GGGATAGCAAGCCAGGAGGTTTAGTACCGCCA
C6	CCCTCAGAACCGCCACCCTCCTATTTTCGGAACCTATTATT
C7	CTGAAACATGAAAGTATTAAGGTCAAGTGCCTTG
C8	AGTAACAGTGCCCGAGAACCACCAGGCGCCACCCTC
C9	AGAACCGCCAGGTGAATTATCACCGTACCGACTAGGGCGACATT
C10	CAACCGATTGATCAGAGGGTAATTGAGCGCTAATATTAGCAGCCTTAC
C11	AGAGAGAATAACATGAACAAGAAAAATAATATCCCATCCTAATT
Region D	
D1	TACGAGCATGTAGAAACCAATCAATAATCGTTTTTTGTTTAACG
D2	TCAAAAATGAAACAGAGAGATAACCCACAAGAATTGAGTTTACCAGCG
D3	CCAAAGACAAATGAGCCATTTGGGAAACCGCCTCC
D4	CTCAGAGCCAGCGCCGCCAGCATTGACAGGAGGTTGAGCCAGAGCCA
D5	CCACCGGATTAGAGCCAGCAAAATCACCAGTAGACAATCAATAGA
D6	AAATTCATATGGTTAAGCCCAATAAAGAGCAAGATATTTATCCCAATC
D7	CAAATAAGAAACGAGCTGTCTTTCCTTATCATTCCAAGAACGGG
D8	TAAAGTACGGTGTCTGGAAGTTTCATTCCAGAATCCCCCTCAA
D9	TGCTTTAAACAGTGAAAAATCTACGTTAATAAAACGAAAGGACAGATGA
D10	ACGGGTGACAGATACGTAATGCCACTATACCGATA
D11	GTTGCGCCGATTTTGCTAAACAACTTTCAACAGTTTCAGATTTCTTAA
D12	ACAGCTTGACGAAGGCACCAACCTAAAACGAAAACCGAACTGACC
D13	AACCTTGAAAGCTAACGGAACAACATTATTACAGGTTACTGCGGAATCGT
D14	CATAAATATTCATTTATAACAGTTGATTCCCAATTCTGCGAACG
Region E	
E1	TATTAACCAAGTACCGCACTCATCGAGAATTGCCAGTTACAAA
E2	ATAAACAGCCATATAACATGAAATAGCAATAGCTATCTCCACGGAATAA
E3	GTTTTATTTTGTCACCATTACCATTAGAATCAAAA
E4	TCACCGGAAGCAGGTCAGACGATTGTGTACTGGTAA
E5	TAAGTTTTAACGGGAGGCTGAGACTCCTCAAGA
E6	GAAGGATTAGGATTAGCGGGATACATGGCTTTT
E7	GATGATACAGGAGGCCTTGATATTCACCGTTTGCCA
E8	TCTTTTCATCAAGGCCGGAAACGTACCAATGAAATATAAAAGAA
E9	ACGCAAAGACATACCGAAGCCCTTTTAAAGAAAAGTCTAACGAGCGTCT
E10	TTCCAGAGCCTAATCAAGCAAGCCGTTTTTATTTTCATCGTAGG
Region F	

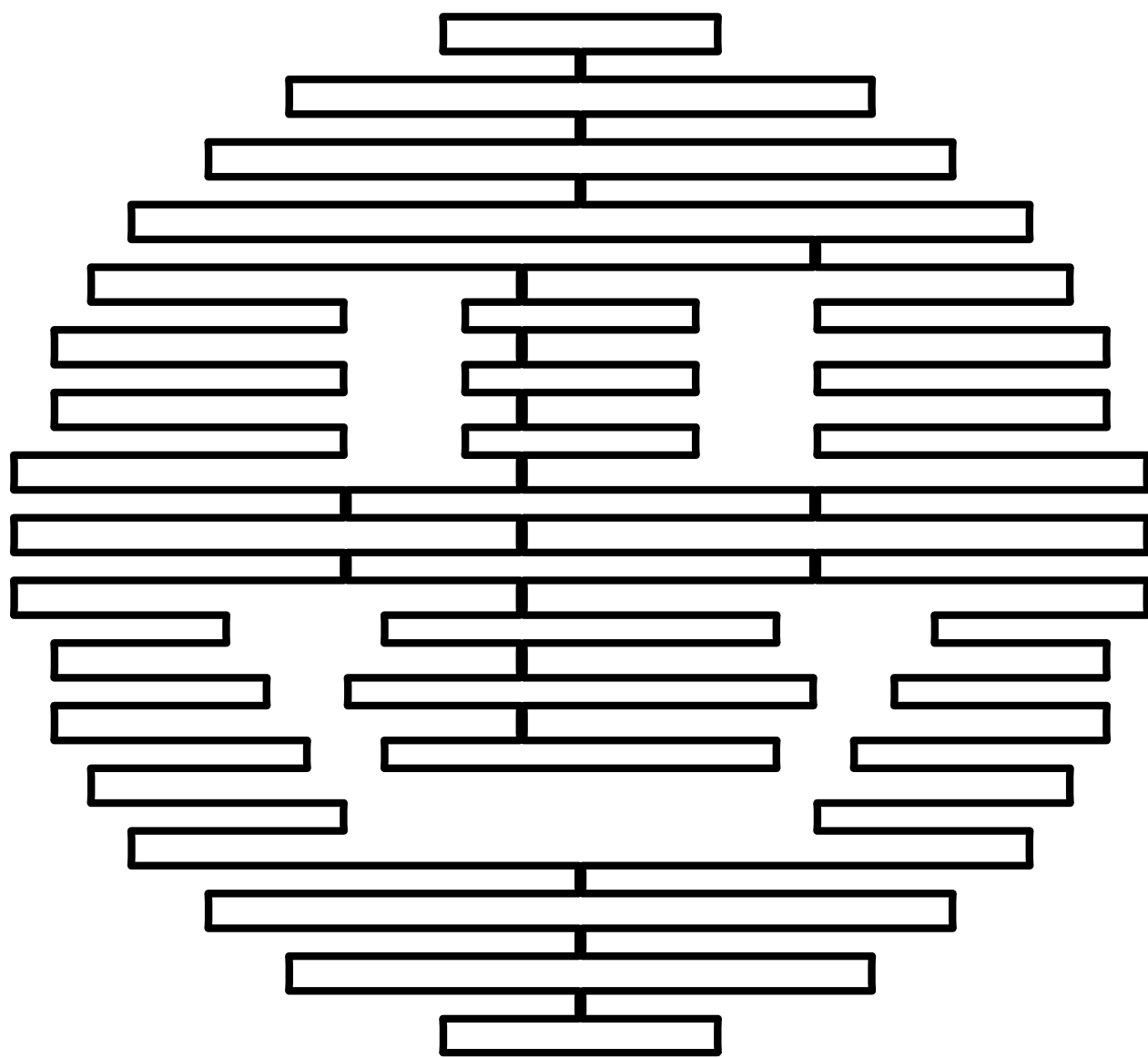
F1	TGGCTTAGAGCTTAATTGCTGAATATAATGAAAATCAGGTCTTT
F2	ACCCTGACTATTATCTTATGCGATTTTAAGAACTGGCTCCCTTCATCAAG
F3	AGTAATCTTGACAAAGACTTTTTTCATGGCCCCACGC
F4	ATAACCGATAGACGTTAGTAAATGCTGAGTTTCGTC
F5	ACCAGTACAAACTTTGATATAAGTATAGCCCGG
F6	AATAGGTGTATCACCGTACTCAATAGGAACCCA
F7	TGTACCGTAACAAATTTTCTGTATGGGACAATGACA
F8	ACAACCATCAGGAAGTTTCCATTAAACGGGTAAAACCAGGCGCAT
F9	AGGCTGGCTGAATTATACCAGTCAGGACGTTGGGAATCAGAAAACGAGA
F10	ATGACCATAAATCACTGTAGCTCAACATGTTTTAAATATGCAAC
Region G	
G1	AATCATTACCGCGCCCAATAGCAAGCAAATACAATTTTATCCTG
G2	AATCTTACCAACGAAGCAGATAGCCGAACAAAGTTACCATACATACATA
G3	AAGGTGGCAACACCATCGATAGCAGCTCATAGCCC
G4	CCTTATTAGAAACAAATAAATCCTCATTAAAGCCAGAATTTTCATCGGC
G5	ATTTTCGGACCGTAATCAGTAGCGACAGAATCACAGTATGTTAGC
G6	AAACGTAGAAAAGAAGGAAACCGAGGAAACGCAATAAAGATTAGTTGCTA
G7	TTTTGCACCCAGCTCAGATATAGAAGGCTTATCCGGTATTCTAAGAACG
G8	CGAGGCGTTTTAGCGAACCTCCCGAAAAGCGAACCAGACCGGAAGCAAAC
G9	TCCAACAGGTCAGGATTAGAGAGTACCTTTAATTGAAGATTAGAGGAA
G10	GCCCGAAAGACTTTAAATTGGGCTTGAGATGGTTTAAATCAACGTAA
G11	CAAAGCTGCTCCGGAACGAGGGTAGCCTTGACGGG
G12	AGTTAAAGCGCTAACGATCTAAAGTTTTGTCGTCTTTCCATATTCGGT
G13	CGCTGAGGAACGGCTACAGAGGCTTTGAGGACTAAGAACCGGATA
G14	TTCATTACCCATTCAACTTTAATCATTGTGAATTACAGTCAGAAGCAAAG
G15	CGGATTGCATCAAACCTCCTTTTGATAAGAGGTCATTTTTGCGGA
Region H	
H1	TTAATTCGAGCTTCCTTGCGGGAGGTTT
H2	TGAAGCCTTAAATCATAACGGAATAC
H3	CCAAAAGAACTGGTGACGAGAAACAC
H4	CAGAACGAGTAGCAAAATATCGCGTT
H5	CTCCTTATTACGAGTTTGCTTTAGCGCACCCCTCAGCAGC
H6	GAAAGACAGCATATTCAGTGAATAAGGCTTGCCCCATGATTAAGA
H7	CGGGATCGTTCAGACTGTAGCGCGTTGGAAAGC
H8	GCAGTCTCAGCCCTCATAGTTAGCCGCTTTTG
H9	GCATTCCACAGACTGAATTTACCGTT
H10	CCAGTAAGCGTCGTTTTGCTCAGTACCAGGCG
H11	GATAAGTGCCGTCGAGAGGGACAACGCCTGTA

* Staples are listed 5’ to 3’ and correspond to the regions and staple numbers shown in the schematic in Figures S26 and S27.

- nanobase.org
- Unified Nanotechnology Format

Reverse Engineering

Design File



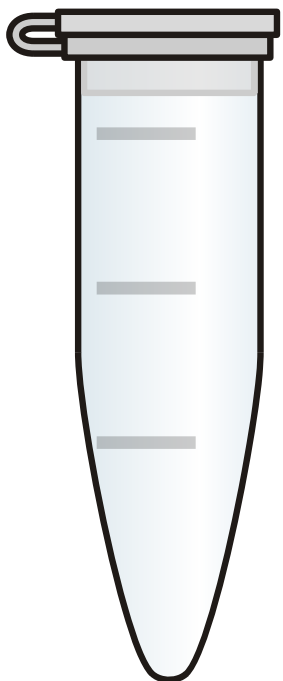
Raw Published Sequences

Scaffold

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GTTCCCTGTCTAAAATCCCTTTAATCGGCCCTCCTGTTTAGCT
CCCGCTCTGATTCTAACGAGGAAAGCACGTTATACGTGCT
CGTCAAAGCAACCATAGTACGCGCCCTGTAGCGGCGCATT
AAGCGCGGCGGGTGTGGTGGTTACGCGCAGCGTGACCG
CTACACTTGCCAGCGCCCTAGCGCCCGCTCCTTTCGCTTT
CTTCCCTTCTTTCTCGCCACGTTGCGCGGCTTTCCCCGT
CAAGCTCTAAATCGGGGGCTCCCTTTAGGGTTCCGATTTA
GTGCTTTACGGCACCTCGACCCCAAAAACTTGATTTGGG
TGATGGTTCACGTAGTGGGCCATCGCCCTGATAGACGGTT
TTTCGCCCTTTGACGTTGGAGTCCACGTTCTTTAATAGTGG
ACTCTTGTTCCAAACTGGAACAACACTCAACCCTATCTCGG
GCTATTCTTTTGATTATAAGGGATTTTGCCGATTTGGAAC
CACCATCAAACAGGATTTTCGCCTGCTGGGGCAAACCAGC
GTGGACCGCTTGCTGCAACTCTCTCAGGGCCAGGCGGTG
AAGGGCAATCAGCTGTTGCCCGTCTCACTGGTGAAAAGAA
AAACCACCCTGGCGCCCAATACGCAAACCGCCTCTCCCC
GCGCGTTGGCCGATTCAATAAT. . .
```

Staples

```
CCGTTGAATTAA
GTCTGTCCATCAGCATAGCAATACTTCTTTGAACTCAAA
AGTAGAAGATTAGTAATAACATCAATCGGAAC
CCTAAAGGTGCCGTAAAGCACTAACTTGCTG
CGAGAAAGGAAGGGAAGCCACCGAGTAAAAGA
CTATCGGCTGGATTATTTACATTGAGGGACAT
AGAACCCTGCTCAATCGTCTGAAACTTGCTGGTAATATCC
AGAACAATATTACCGCATACCTACATTTTGACTCTGACCT
GTGGCACAAAAACGCTCATGGAACAGCCATTGCAACAGG
CAAATATCTAGCCCTAAACATCGAAGAATAC
GAAAGCGTCCATTAAAAATACCGACTAAAGCATCACCTTG
TAGTCTGGCTAT
GACAATATTTTGAATTTAATGCGCGAACTGAAAACCCCTC
GTAATAAAGCAGATTACCAAGTCAATAGGGTT
.
```

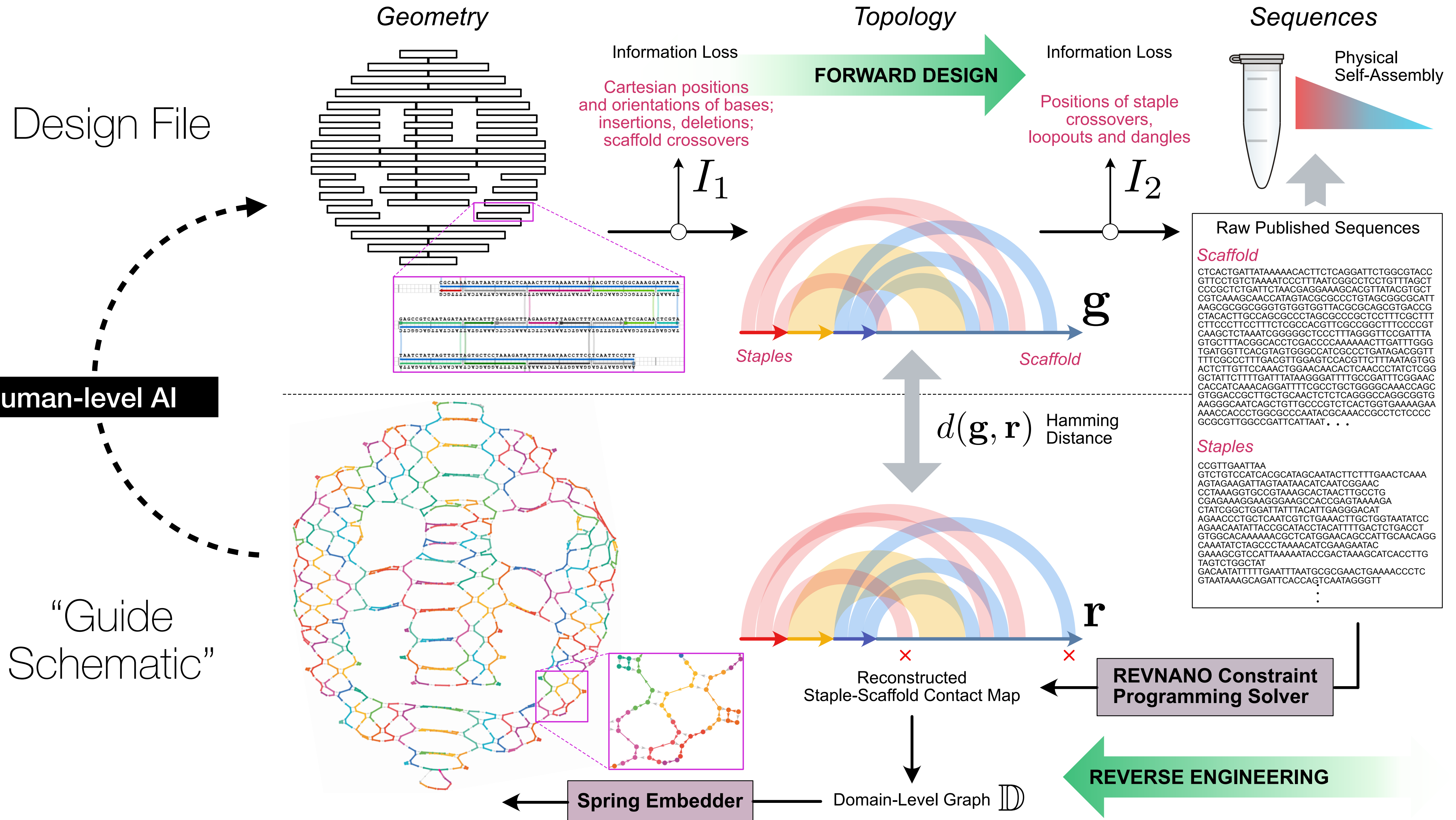


Physical
Self-Assembly



Is the inverse
problem possible?

Reverse Engineering



Reverse Engineering: Why

Help recover
editable
electronic
schematic

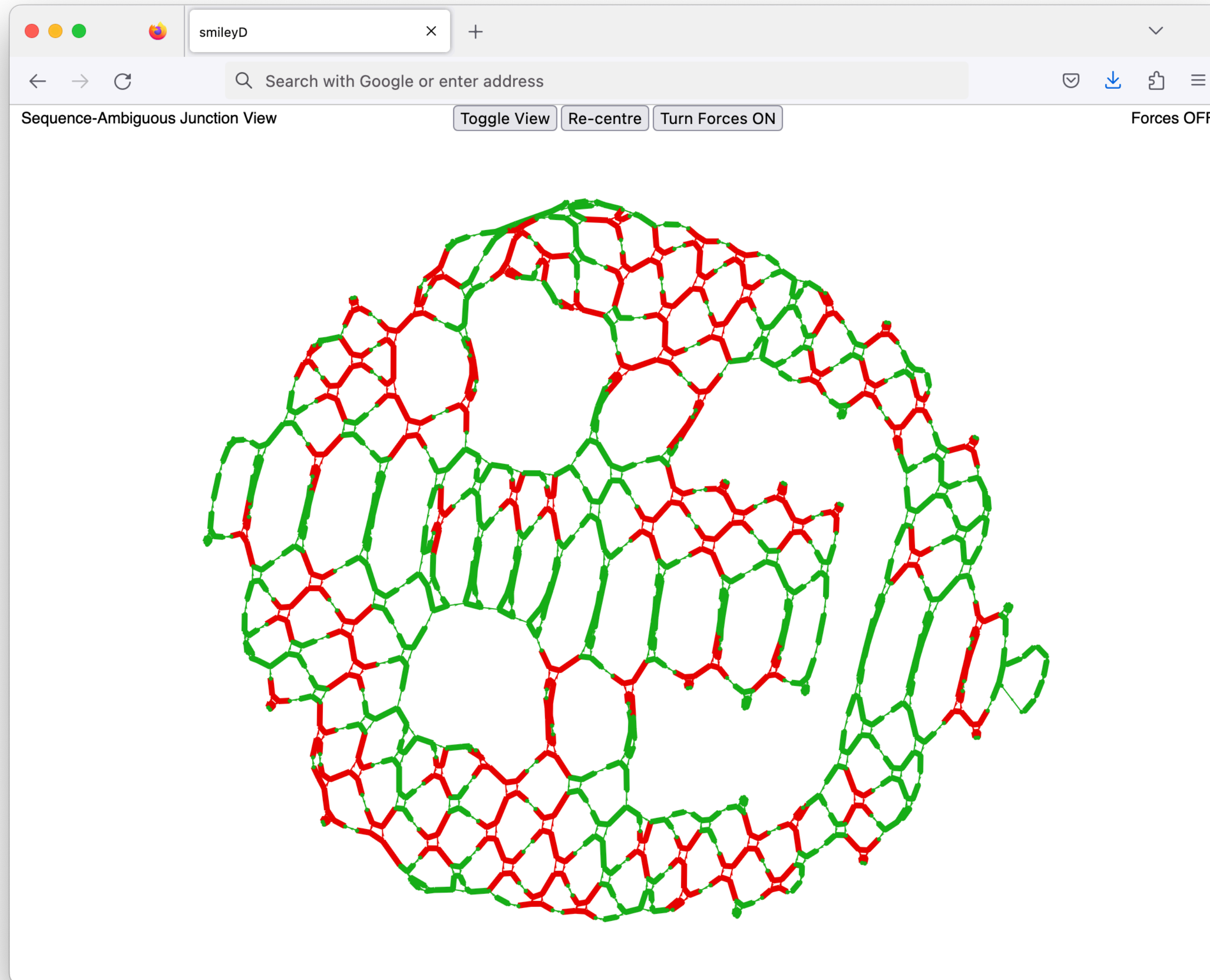
Examine
origami in
greater detail

Double check
no sequence
errors in
published lists

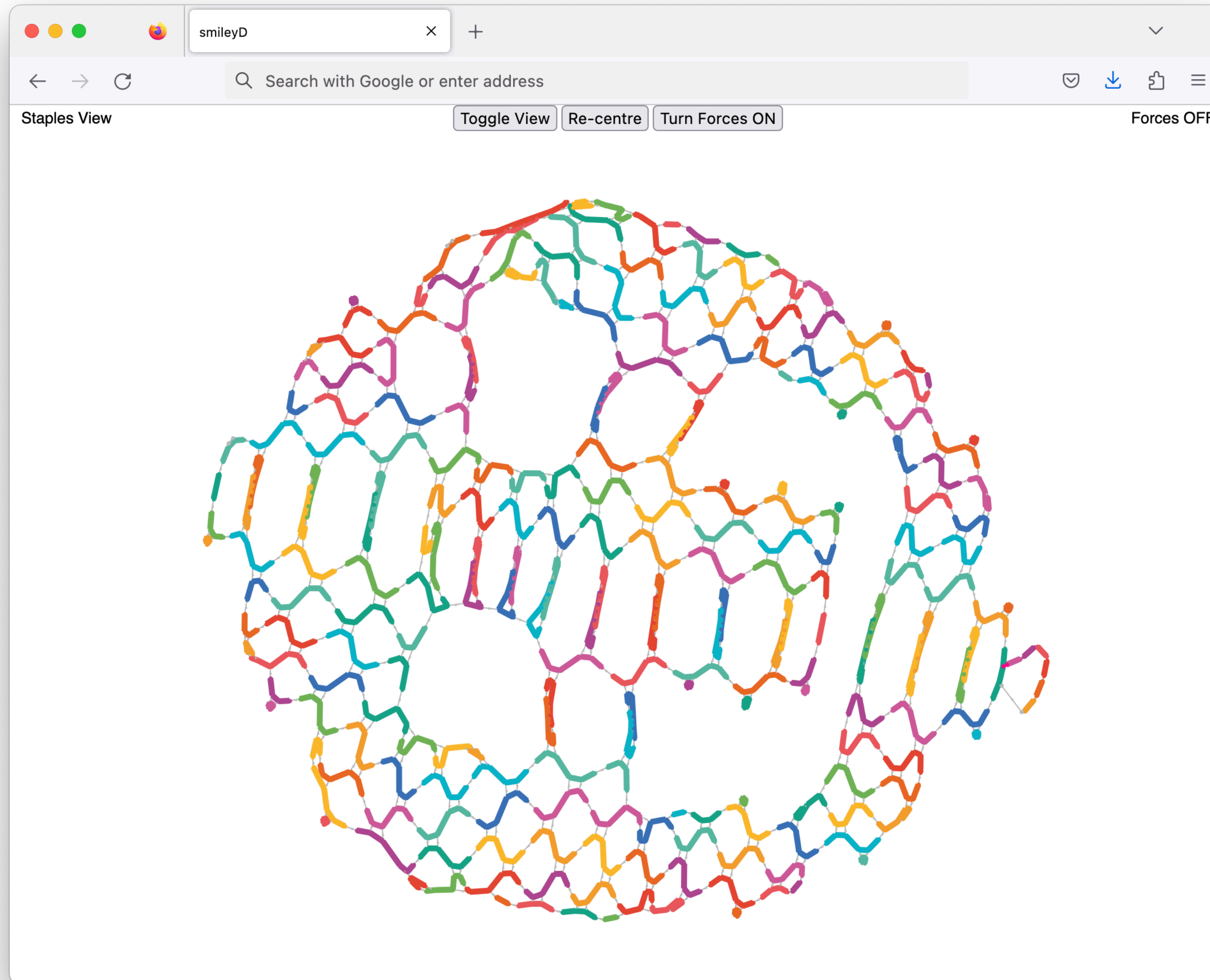
Decide what
scaffold
sequence is
used!

Easy reverse =
less kinetic
traps in
origami folding

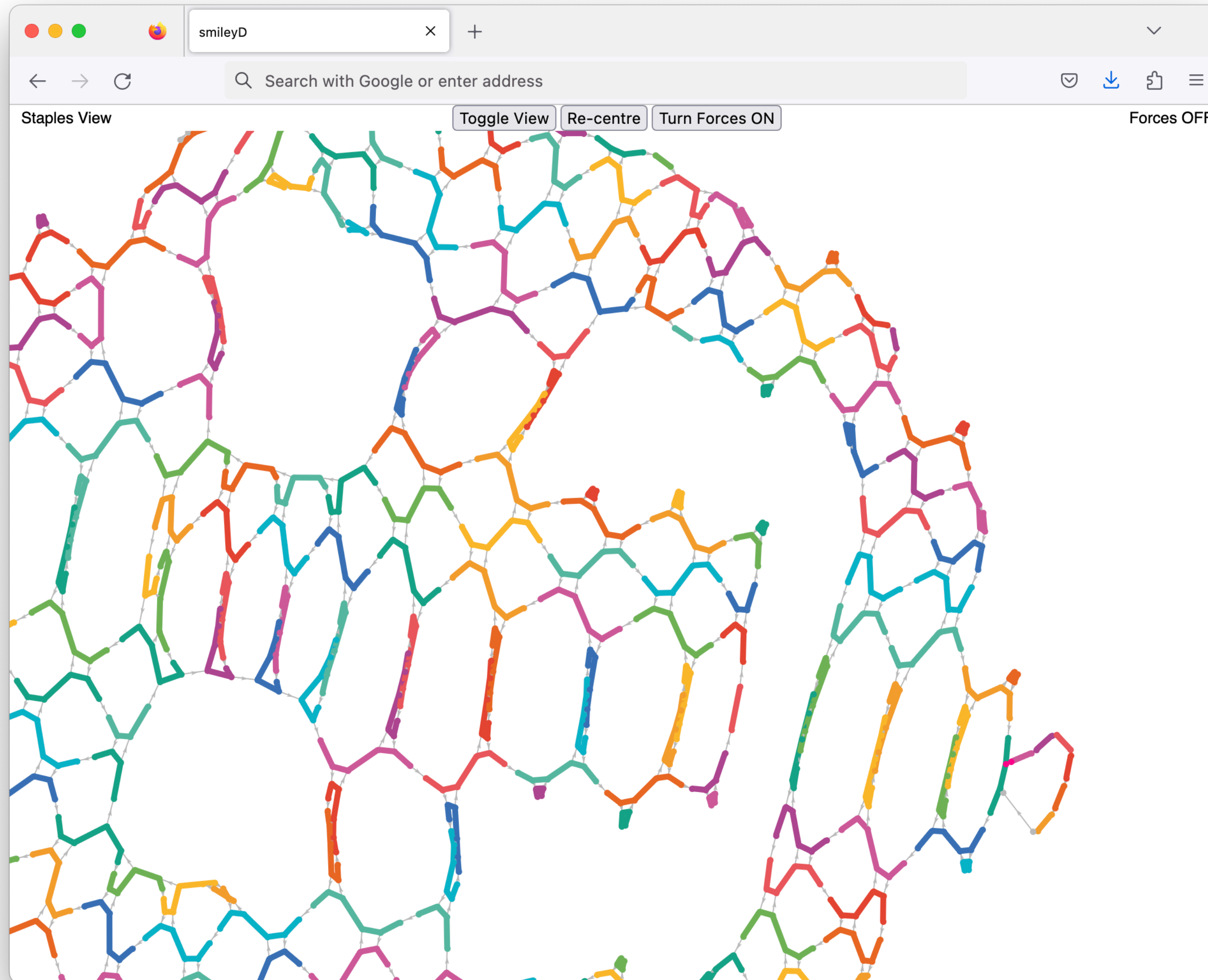
Guide Schematic - Dynamic HTML Page



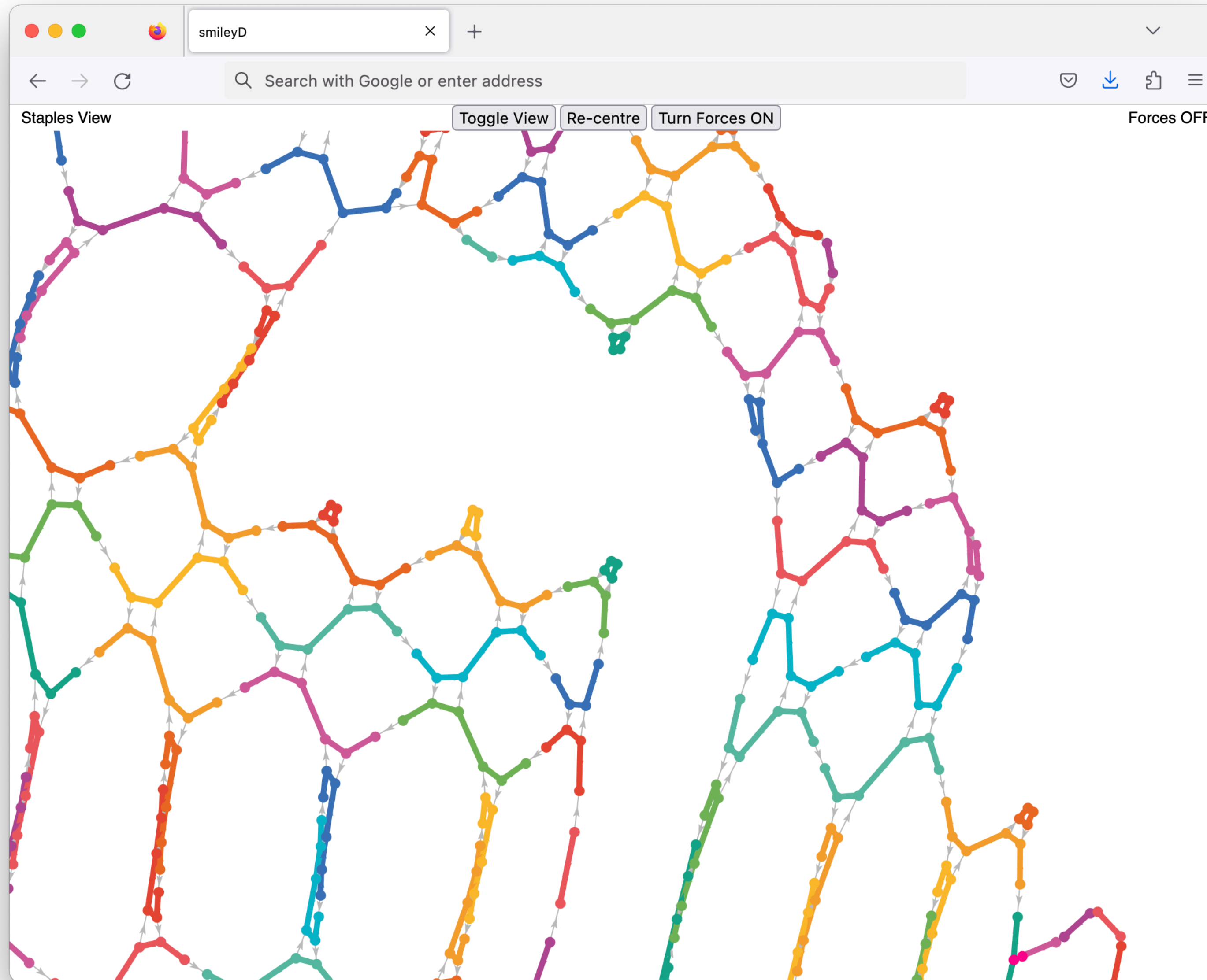
Guide Schematic - Dynamic HTML Page



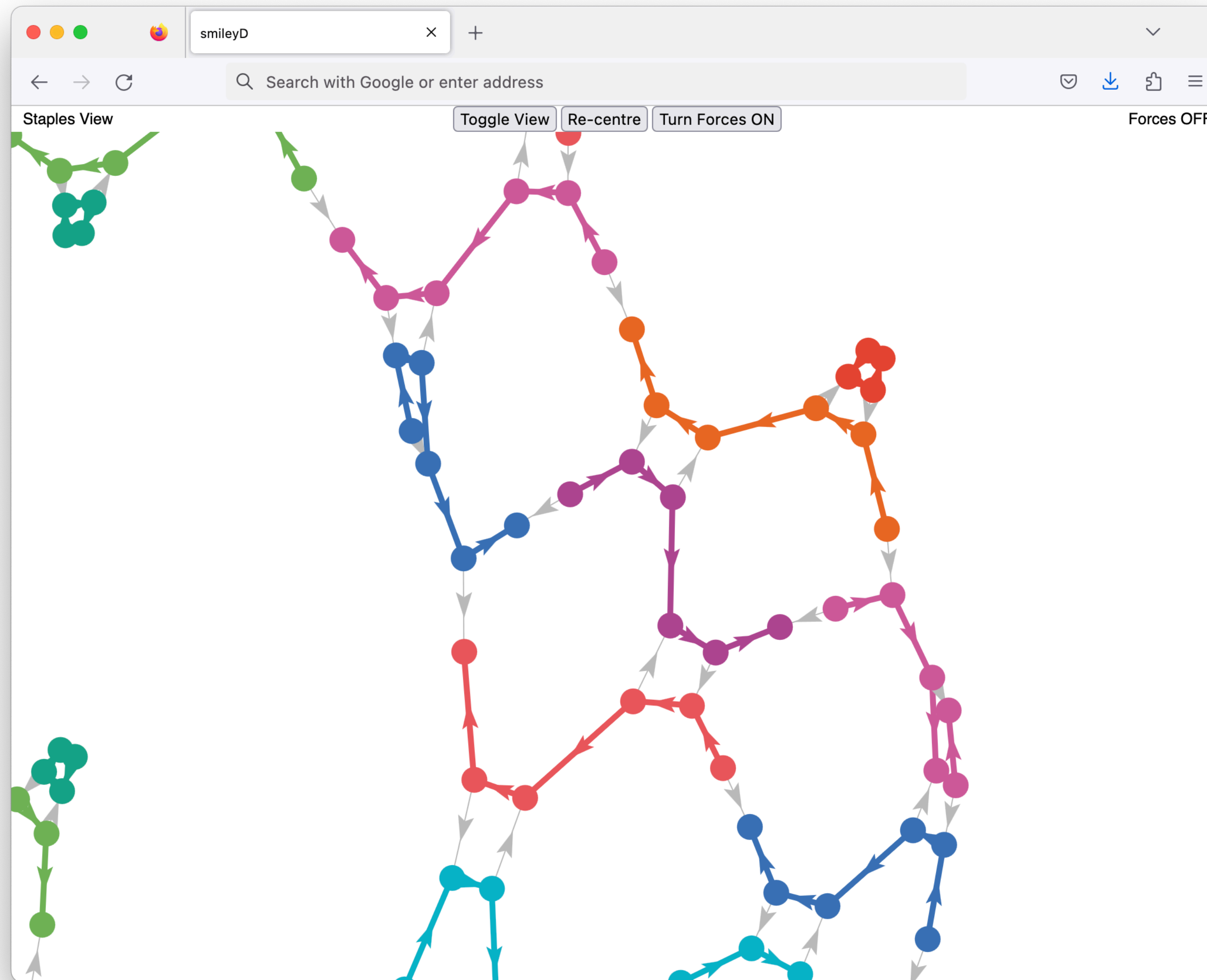
Guide Schematic - Dynamic HTML Page



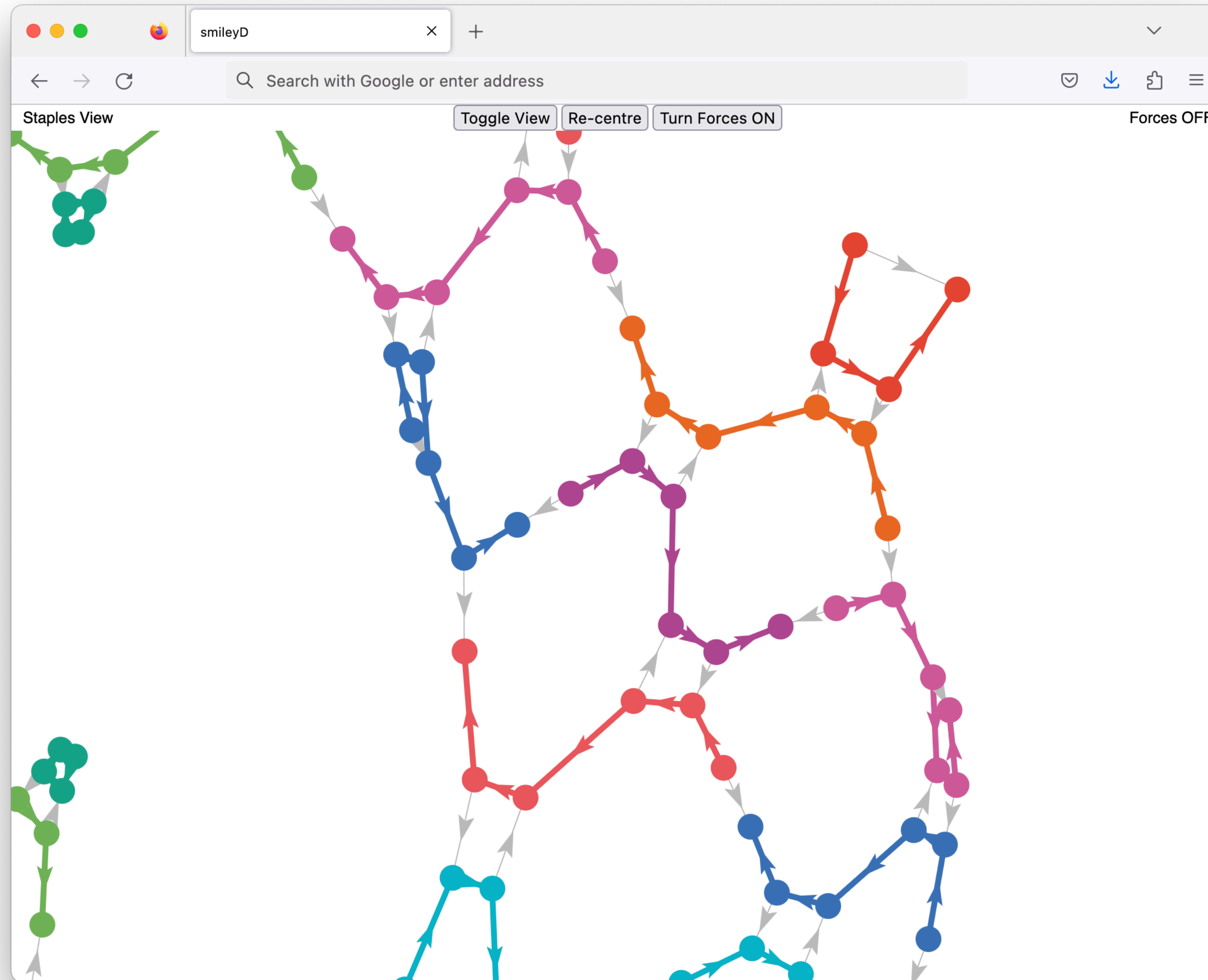
Guide Schematic - Dynamic HTML Page



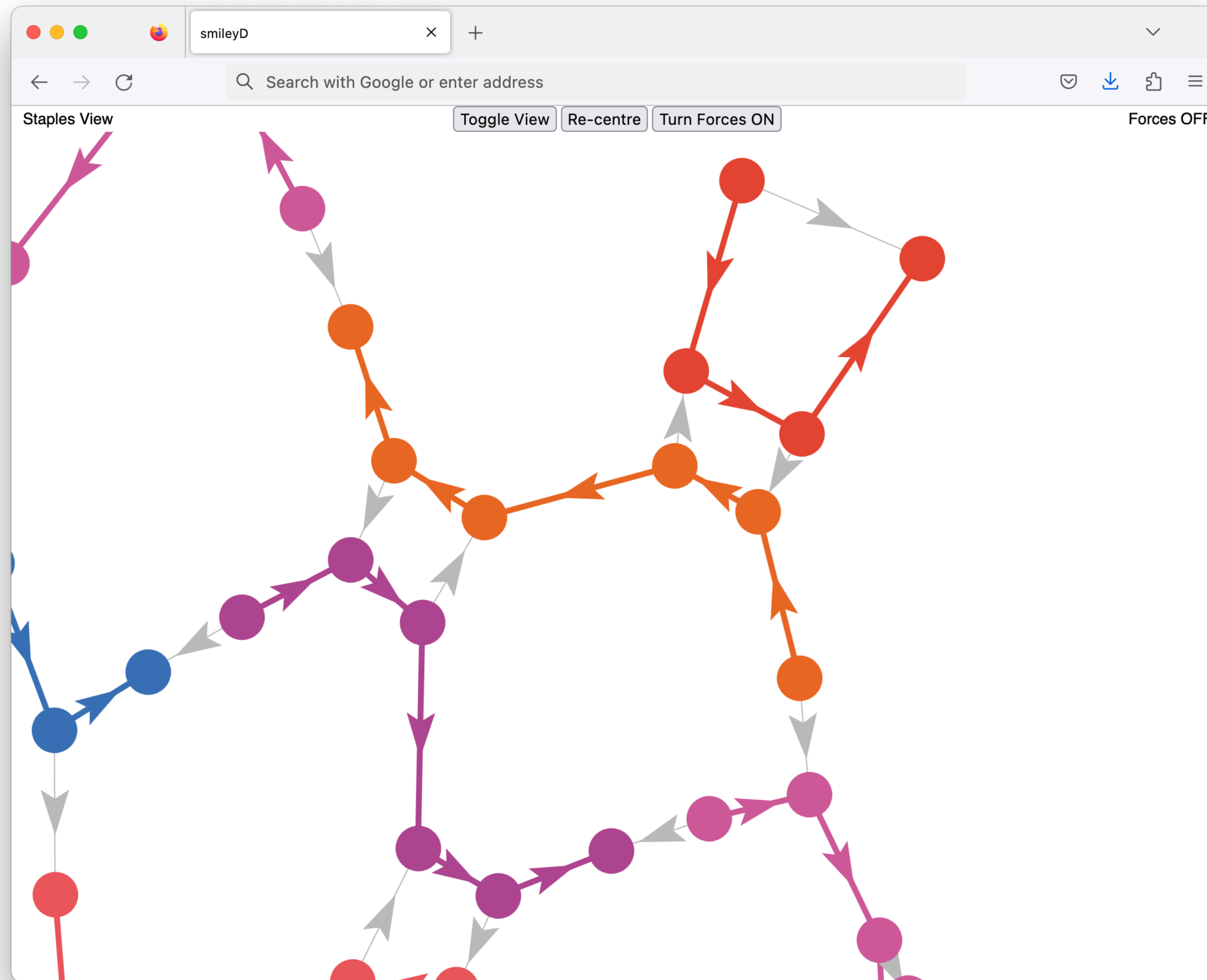
Guide Schematic - Dynamic HTML Page



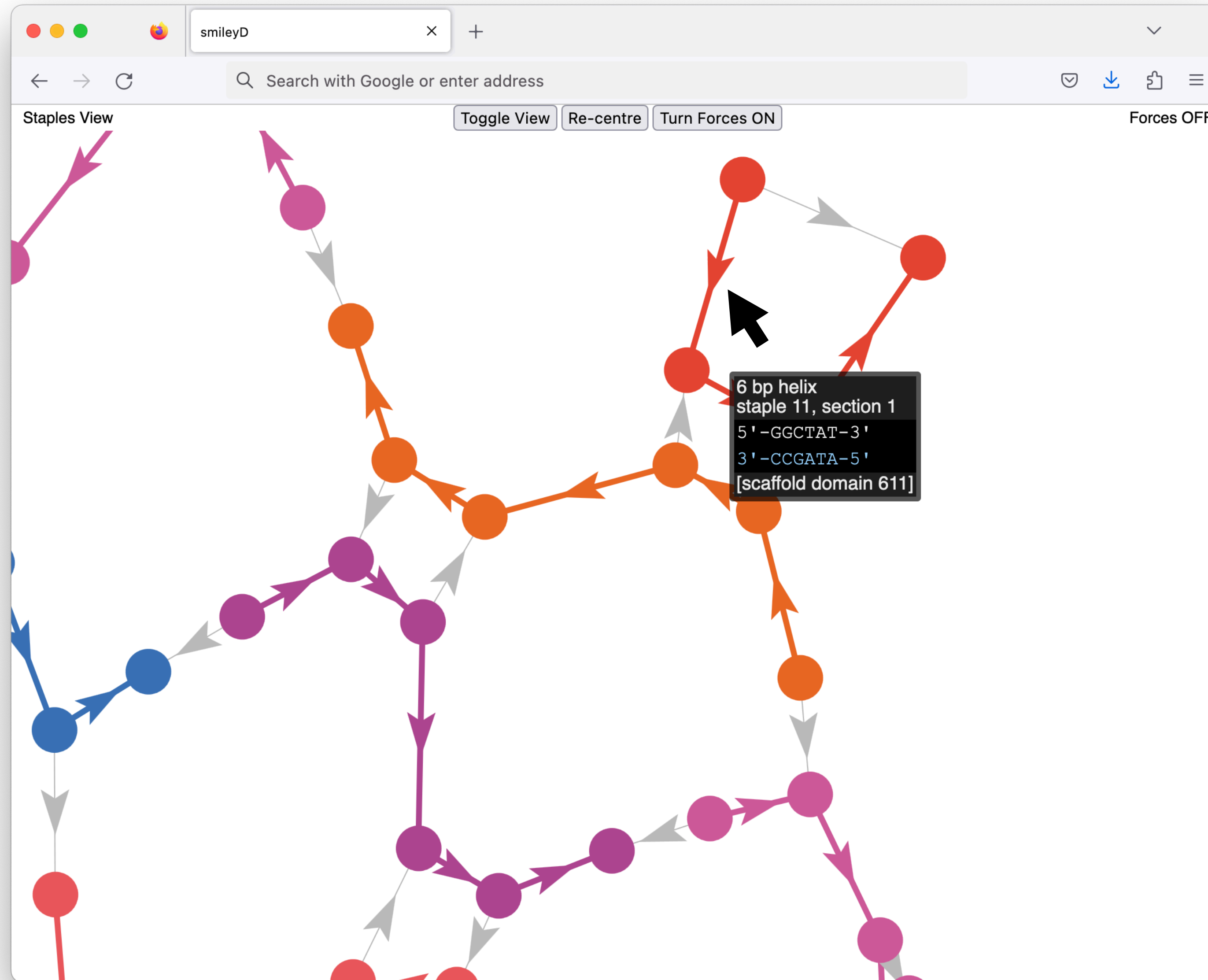
Guide Schematic - Dynamic HTML Page



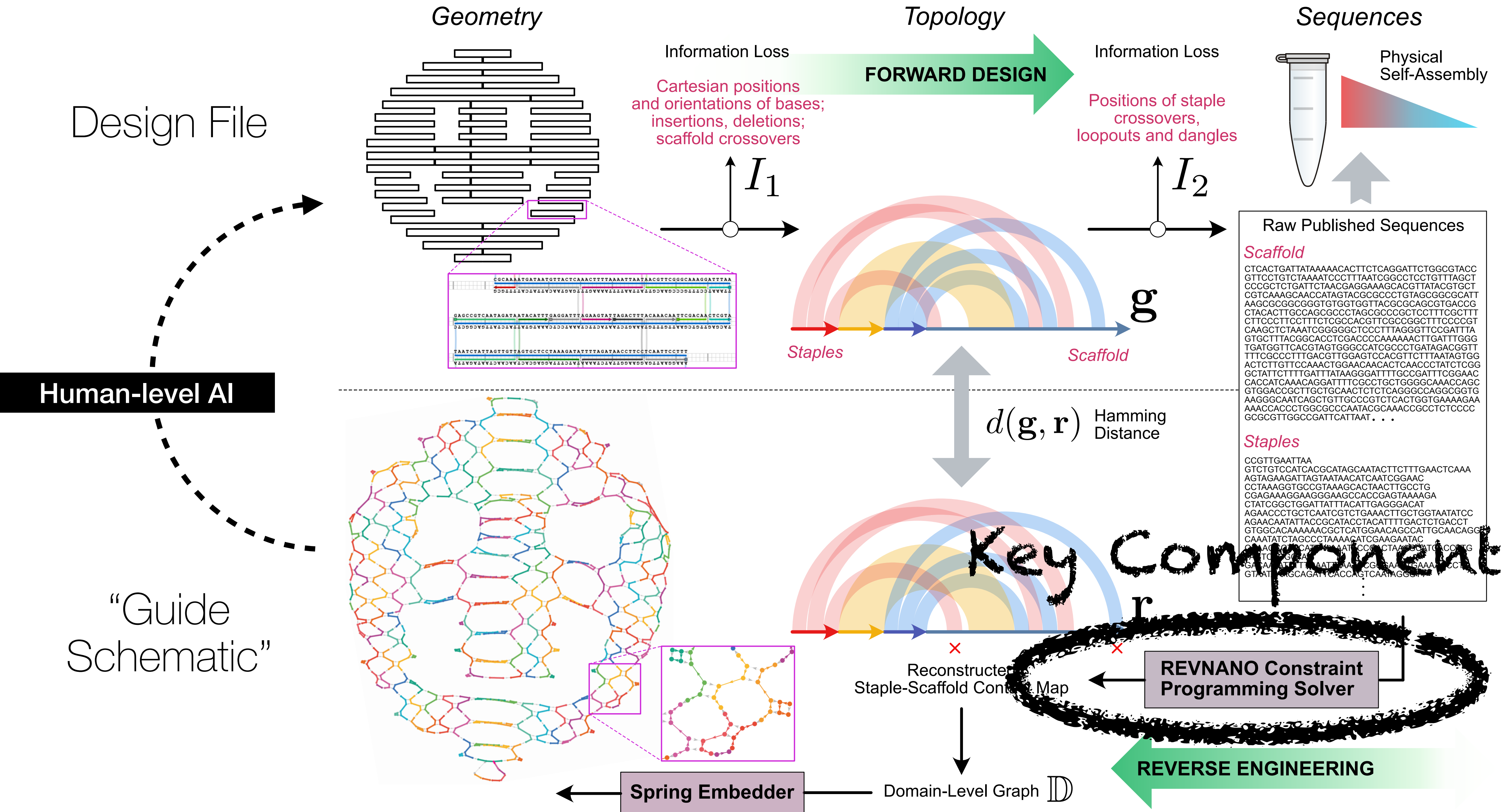
Guide Schematic - Dynamic HTML Page



Guide Schematic - Dynamic HTML Page



Reverse Engineering



Constraint Satisfaction Problems (CSP)

5	3			7				
6			1	9	5			
	9	8					6	
8				6				3
4			8		3			1
7				2				6
	6					2	8	
			4	1	9			5
				8			7	9

Constraint Satisfaction Problems

- Given:
 - A set of **decision variables**.
 - For each decision variable, a **domain** of potential values.
 - A set of **constraints** on the decision variables.
- Find:
 - An **assignment** of values to variables such that all constraints are satisfied.

Constraint Satisfaction Problems (CSP)

5	3			7				
6			1	9	5			
	9	8					6	
8				6				3
4			8		3			1
7				2				6
	6					2	8	
			4	1	9			5
				8			7	9

Constraint Satisfaction Problems

- Given:

- A set of **decision variables**.
- For each decision variable, a **domain** of potential values.
- A set of **constraints** on the decision variables.

- Find:

- An **assignment** of values to variables such that all constraints are satisfied.

Empty squares

1 to 9

Sudoku rules!

Completed
Sudoku square

Constraint Propagation

5	3			7				
6			1	9	5			
	9	8					6	
8				6				3
4			8		3			1
7				2				6
	6					2	8	
			4	1	9			5
				8			7	9

5	3			7				
6			1	9	5			
	9	8					6	
8				6				3
4			8	5	3			1
7				2				6
	6					2	8	
			4	1	9			5
				8			7	9

5	3				7			
6			1	9	5			
	9	8					6	
8				6				3
4			8	5	3			1
7			9	2				6
	6					2	8	
			4	1	9			5
				8			7	9



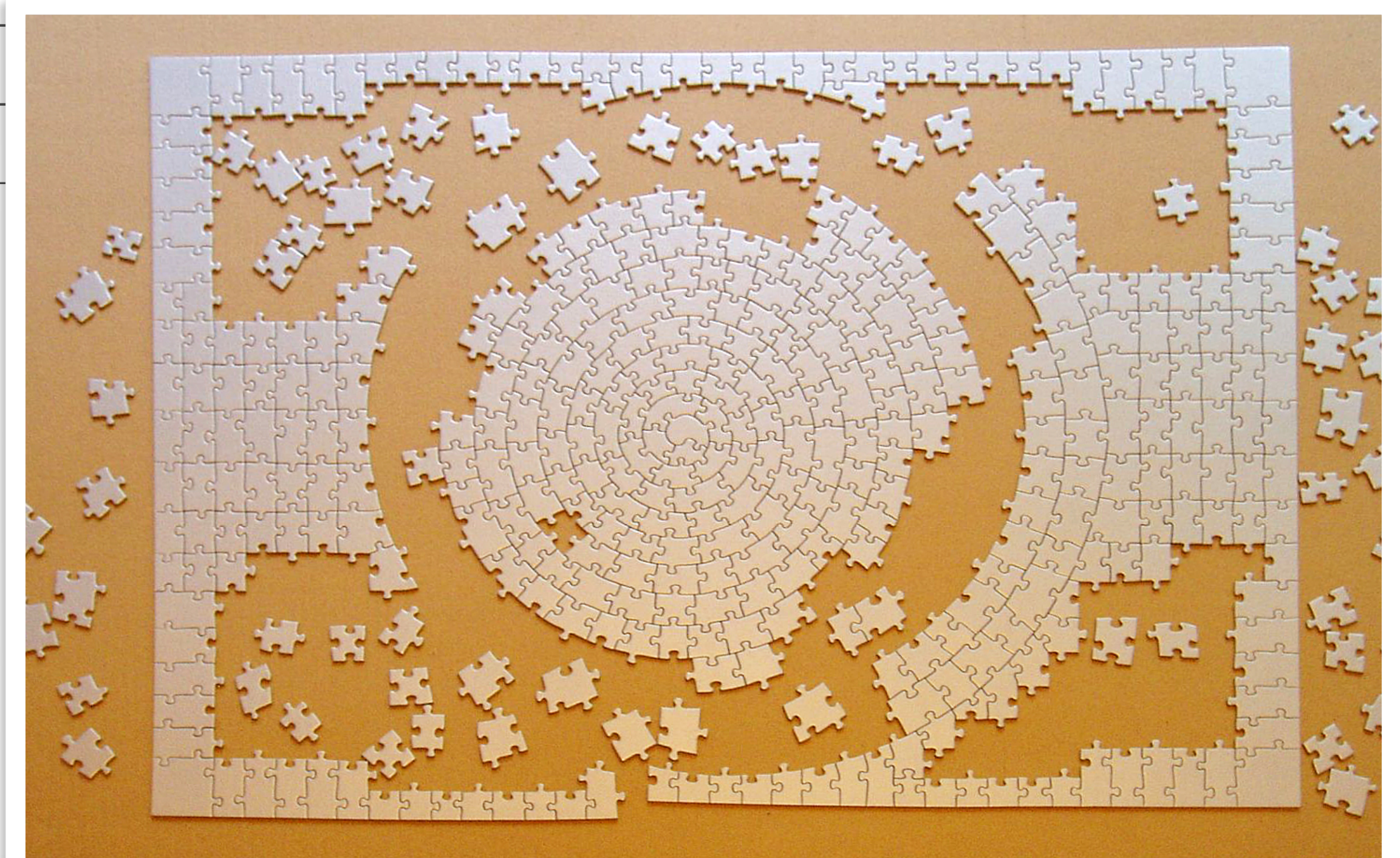
Constraints build iteratively
to systematically narrow down a solution

Constraint Propagation

5	3			7				
6			1	9	5			
	9	8					6	
8				6				3
4			8		3			1
7				2				6
	6					2	8	
			4	1	9			5
				8			7	9

5	3			7				
6			1	9	5			
	9	8					6	
8				6				3
4			8	5	3			1
7				2				6
	6					2	8	

5	3			7				
6			1	9	5			
	9	8					6	
8				6				3
4			8	5	3			1
7			9	2				6
	6					2	8	
								5
								9



Reverse Engineering an Origami Contact Map as a CSP



Constraint Satisfaction Problems

- Given:

- A set of **decision variables**.
- For each decision variable, a **domain** of potential values.
- A set of **constraints** on the decision variables.

- Find:

- An **assignment** of values to variables such that all constraints are satisfied.

Staples

Set of possible
W-C routes
through scaffold

Completed
origami!

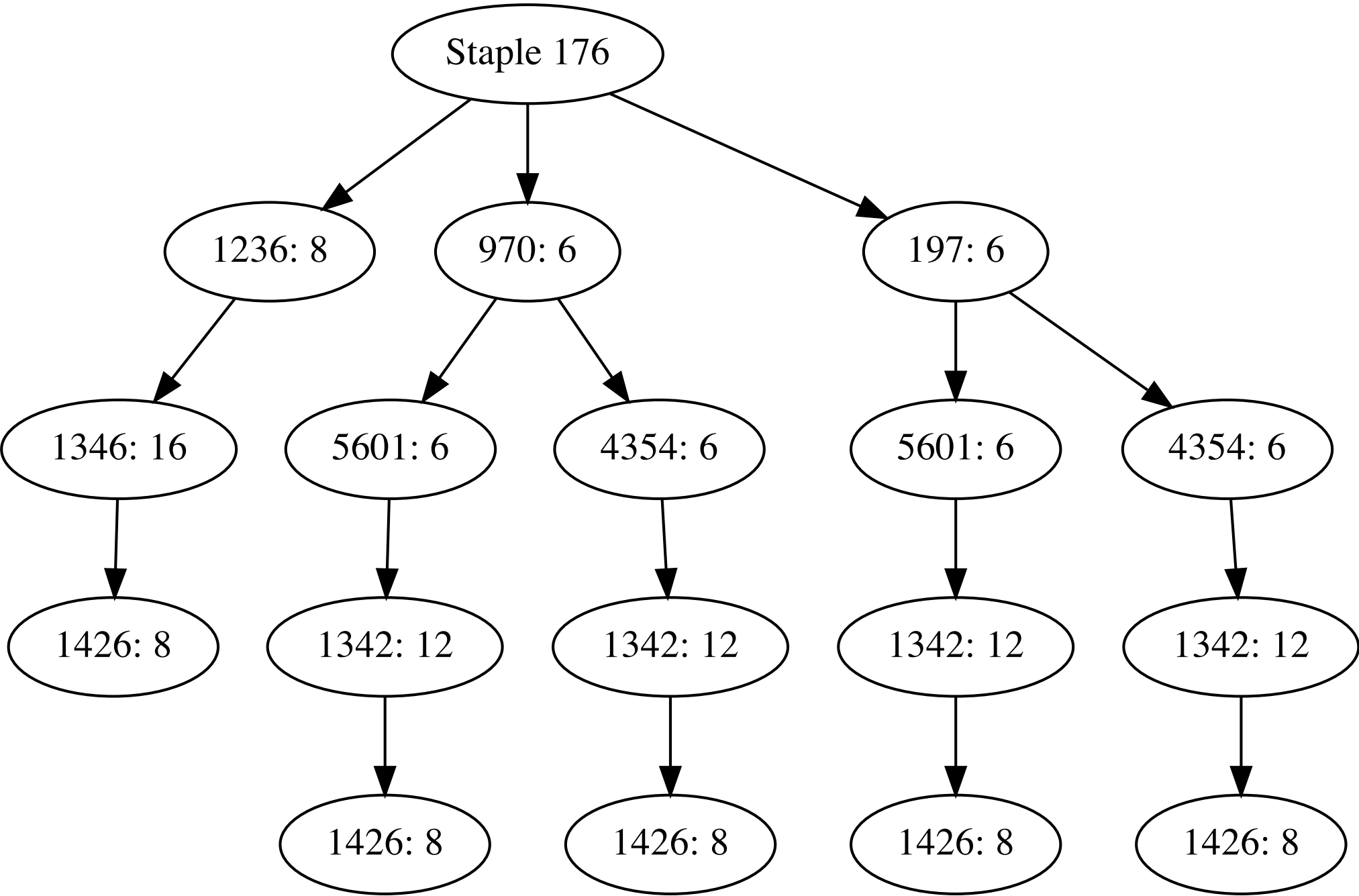
No overlaps, all
staples placed

Rebuilding The Smiley Face From Sequences

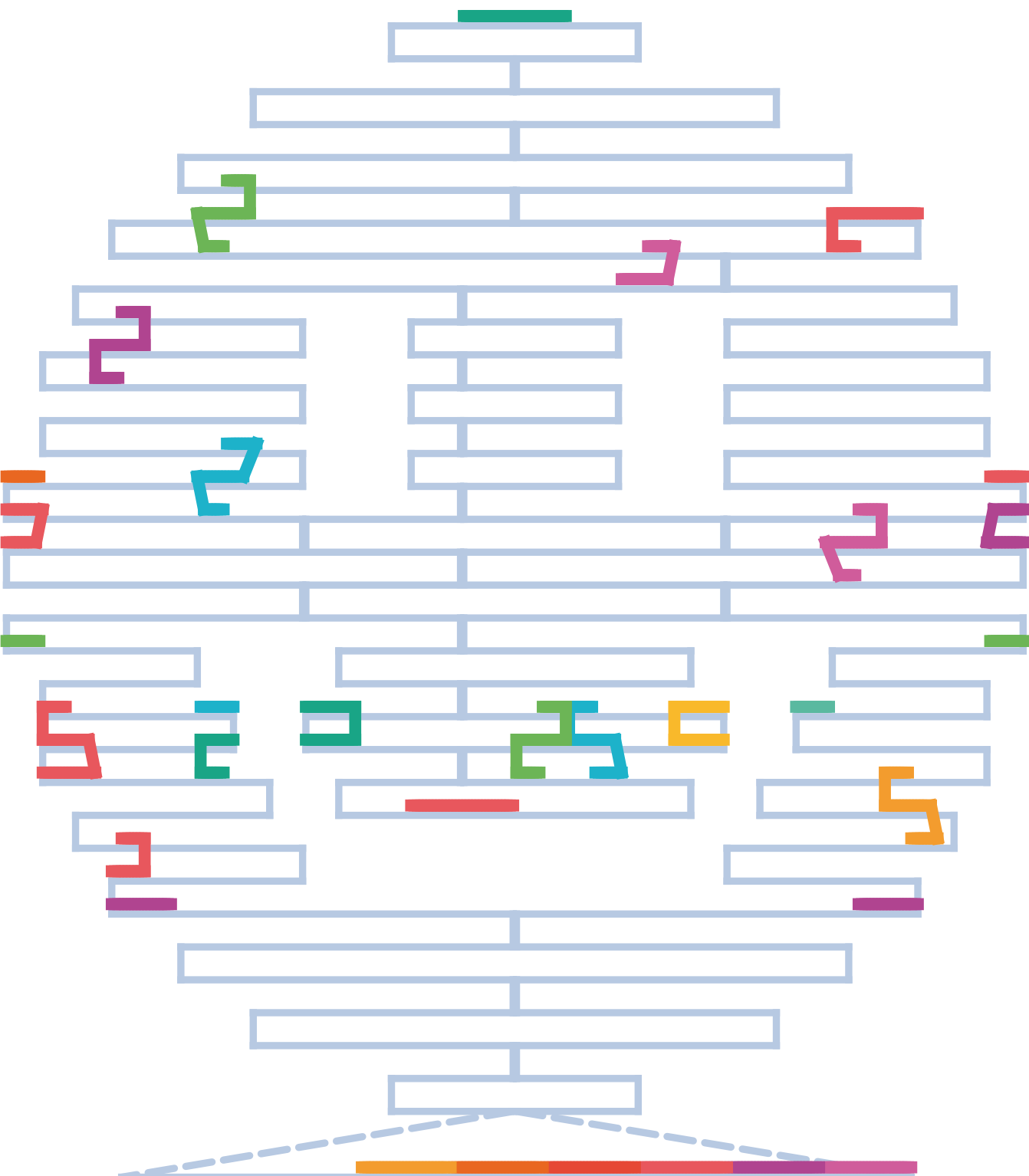
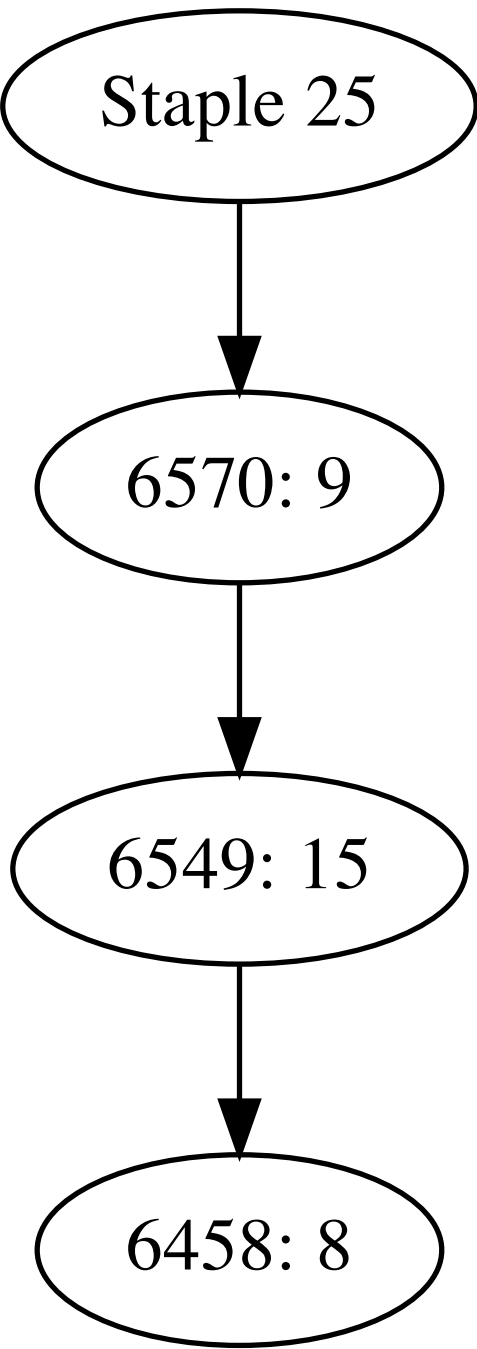
Stage 0: Establish The Initial Hard Constraints

5	3			7				
6			1	9	5			
	9	8					6	
8				6				3
4			8		3			1
7				2				6
	6					2	8	
			4	1	9			5
				8			7	9

Staple with multiple possible routes



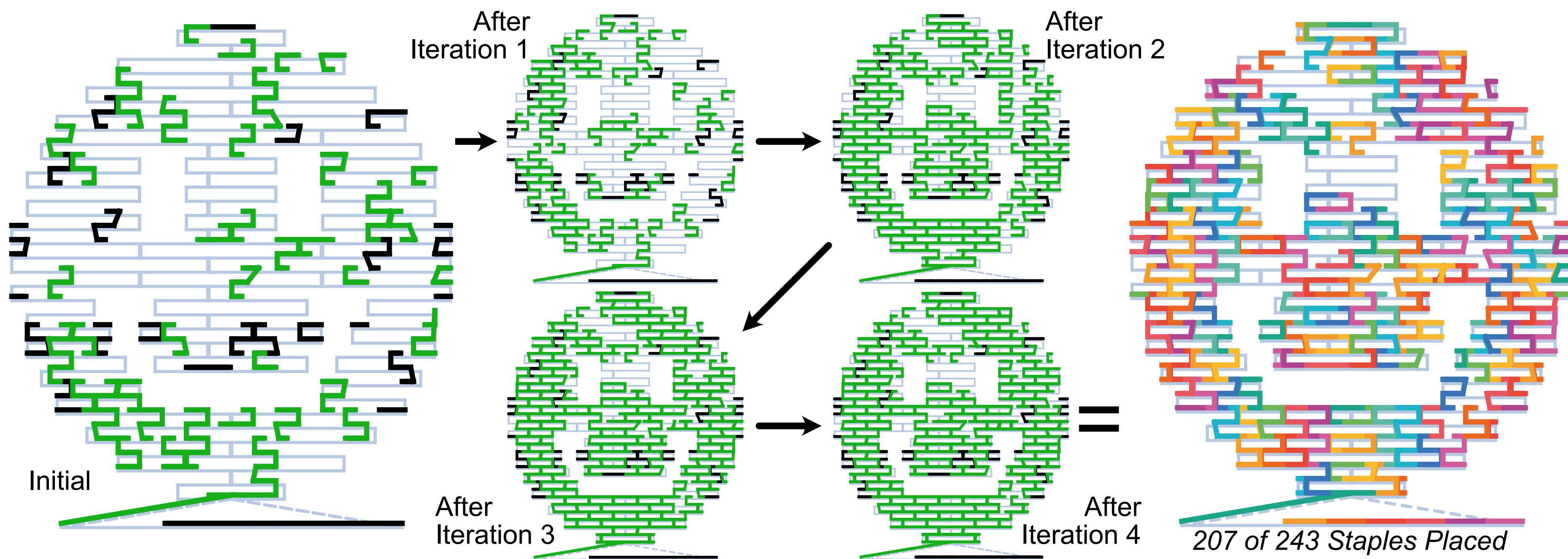
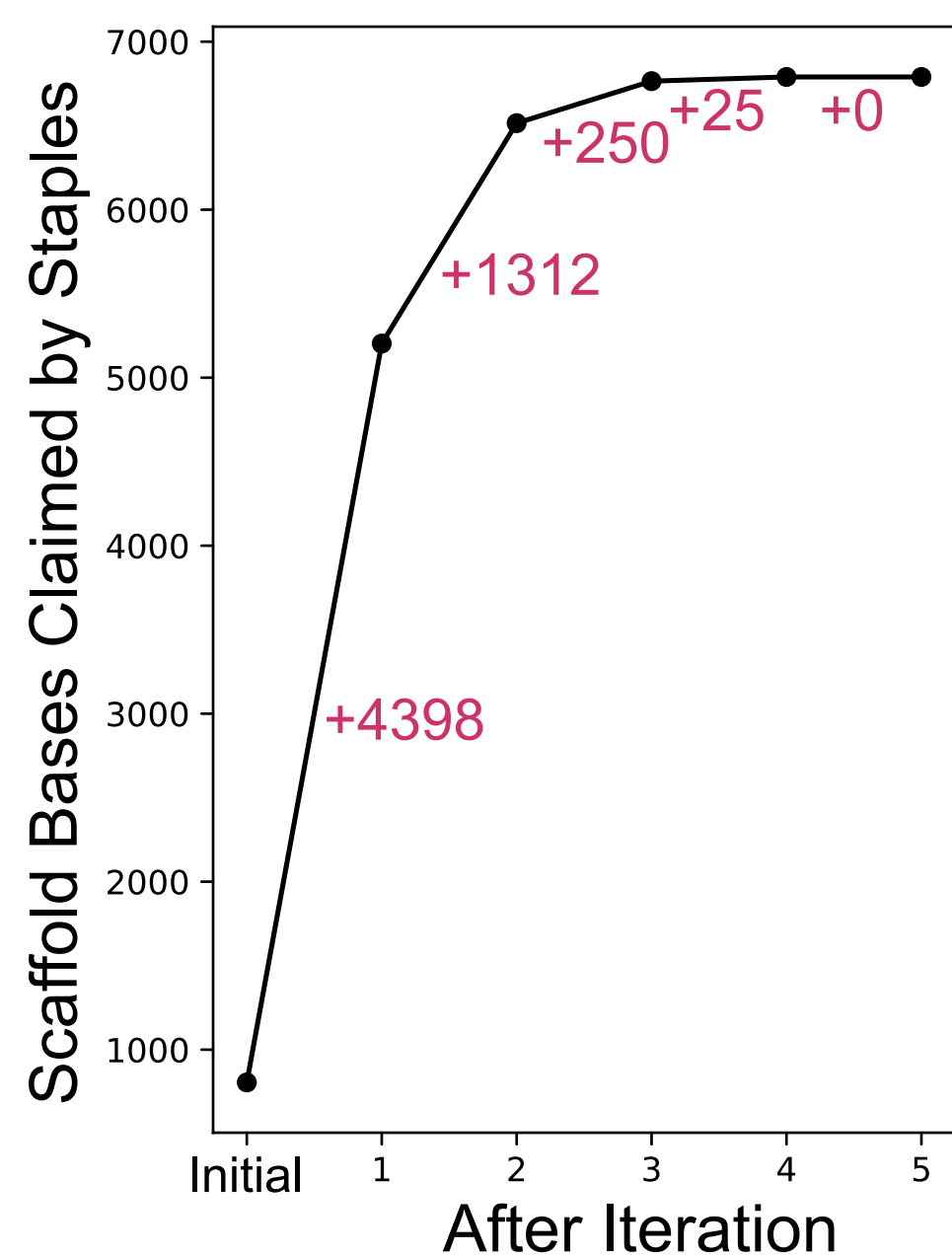
Staple with single route



32 Definite 1-Route Staples Placed

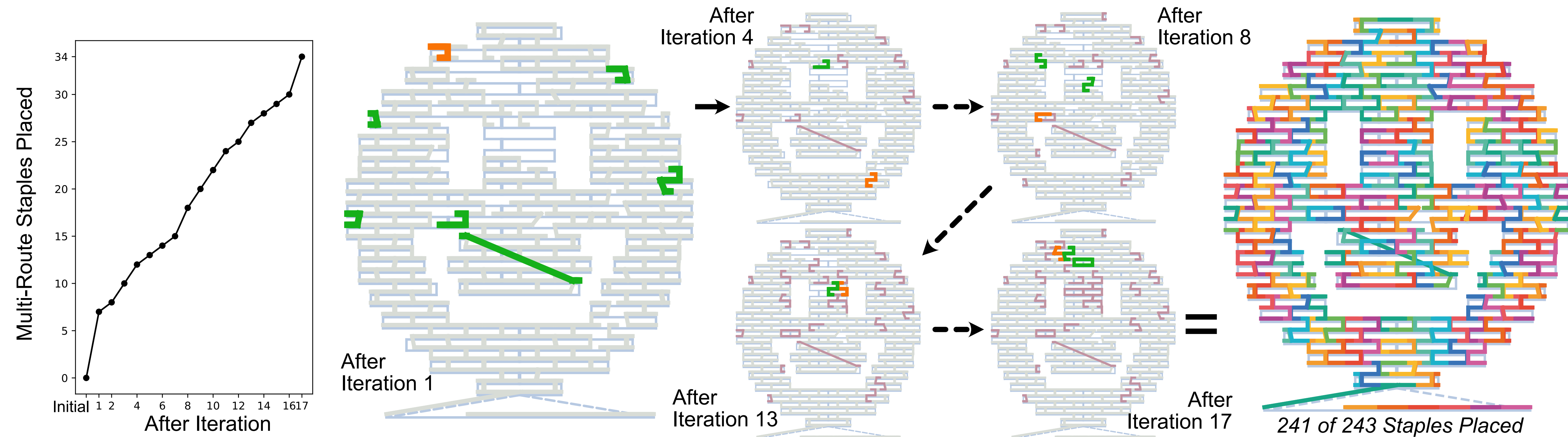
Rebuilding The Smiley Face From Sequences

Stage 1: Constraint Propagation



Rebuilding The Smiley Face From Sequences

Stage 2: Force-Place "Stubborn" Staples by Shortest Path



> 95% staples placed

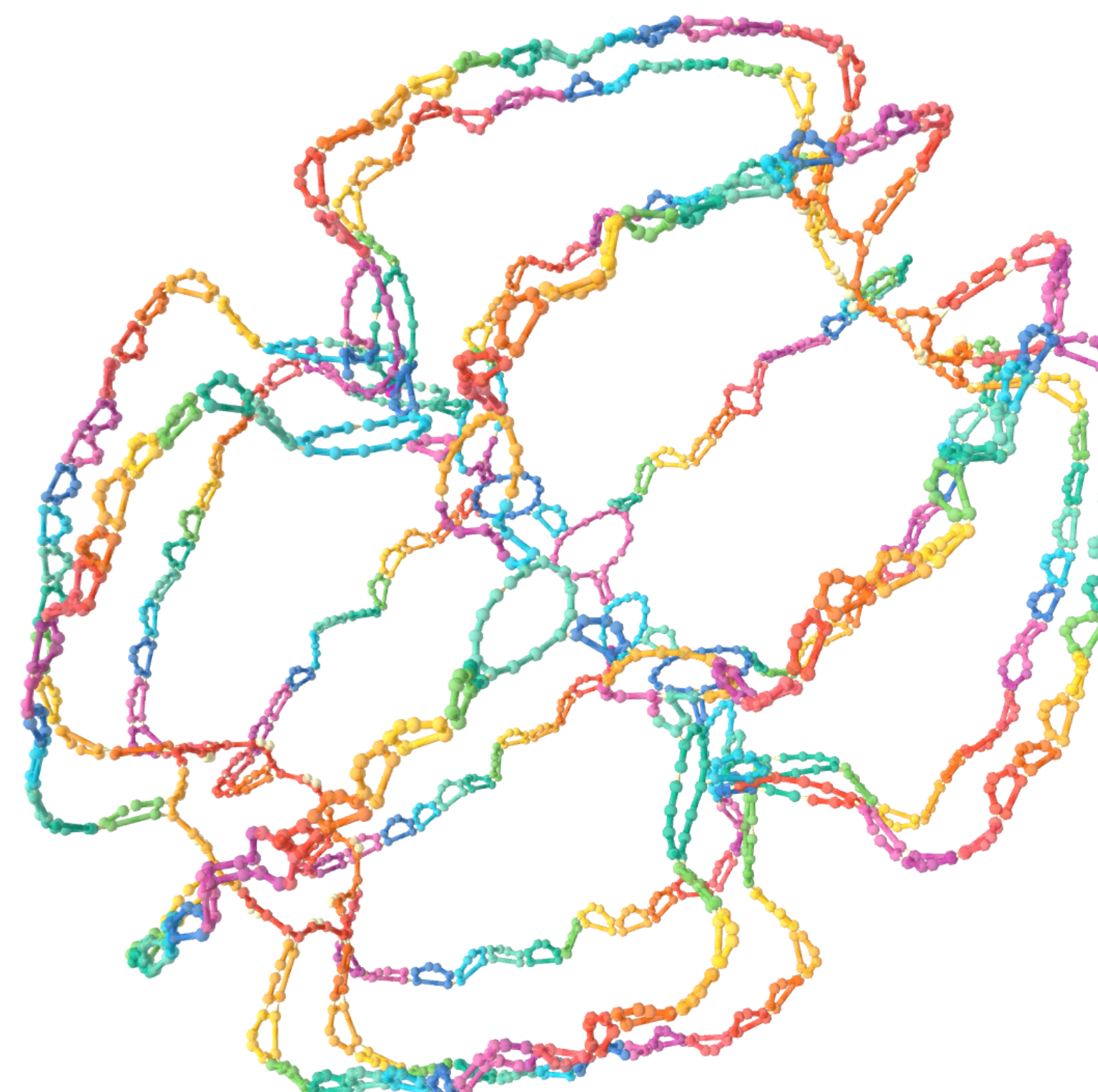
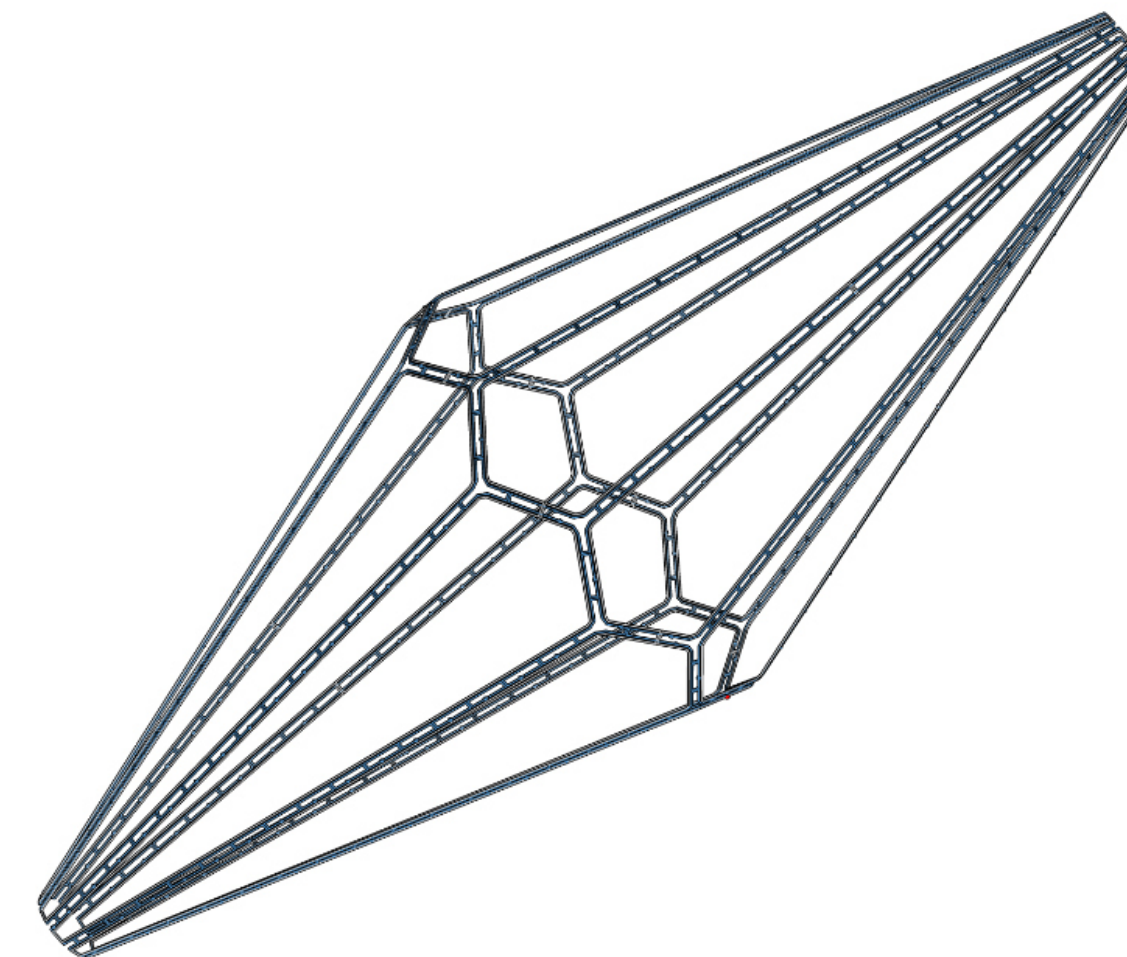
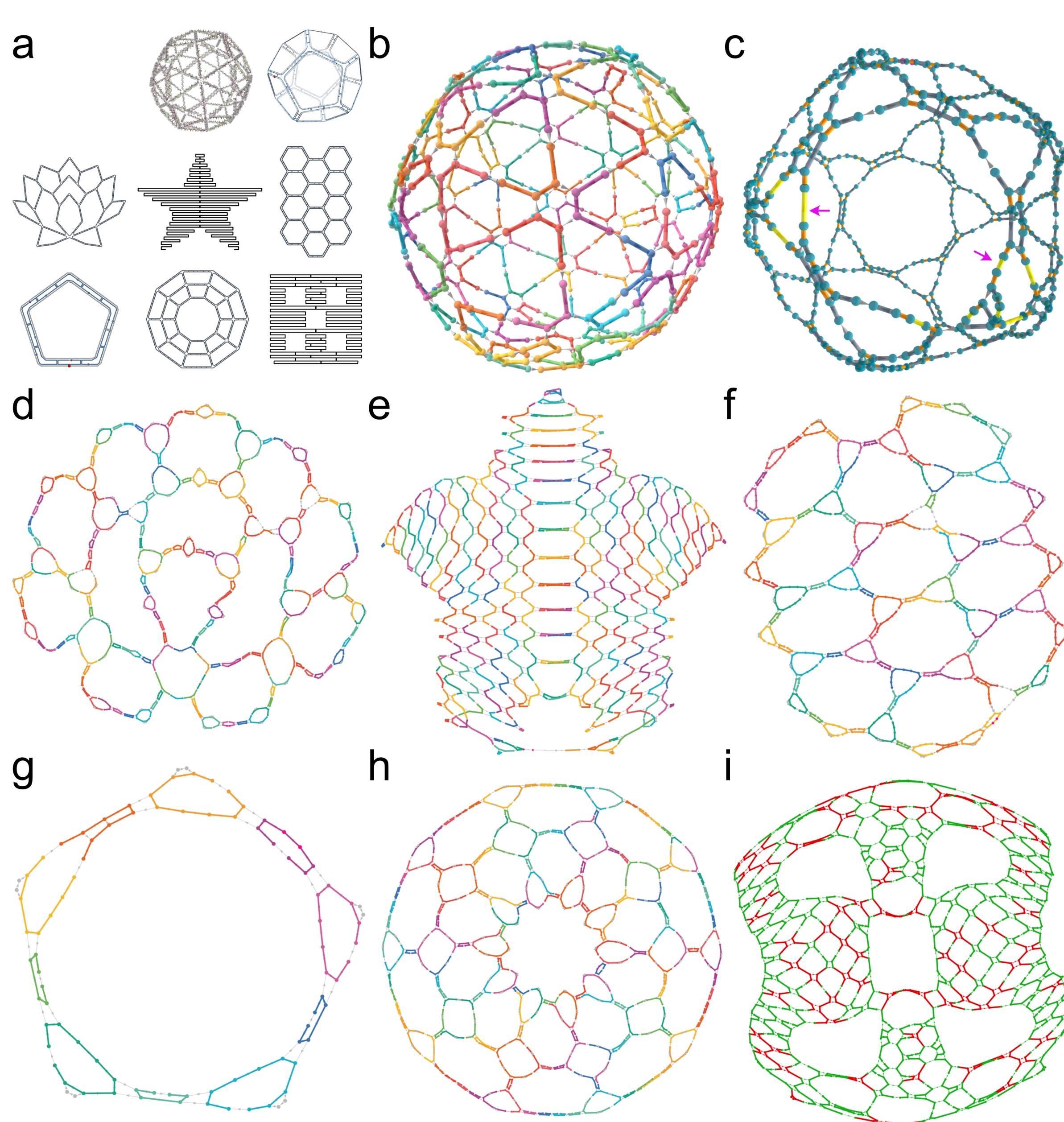
Tested on **36**
DNA origamis
from literature

					NAIVE Solver				REVNANO Solver						
ID	Raster Origami	Ref	Dim	Staples	$\mu_{\min}$	$d(\mathbf{g}, \mathbf{r})$	SP%	Wall(s)	$\mu_{\min}$	σ	β	$d(\mathbf{g}, \mathbf{r})$	SP%	Wall(s)	Vs.
1	RNA/DNA Hybrid Triangle	[24]	2	22	6	16	100.0	< 1	6	0	0.10	16	100.0	< 1	=
2	M1.3 Four Finger	[38]	2	24	6	6	100.0	< 1	6	0	0.05	6	100.0	< 1	=
3	Brick	[39]	3	45	5	459	77.8	< 1	6	1	0.30	332	84.4	< 1	R
4	Mini Triangle	[40]	2	66	6	308	87.9	< 1	6	1	0.05	30	100.0	1	R
5	DeBruijn Sequence Square	[41]	2	70	6	44	100.0	< 1	6	0	0.05	44	100.0	1	=
6	puc19 Rectangle	[33]	2	90	6	2	100.0	< 1	6	0	0.30	2	100.0	1	=
7	6 Helix Bundle	[39]	3	96	–	–	–	–	5	2	0.45	136	96.9	20	R
8	Fivewell Plate	[42]	2	158	–	–	–	–	6	6	0.30	100	100.0	272	R
9	Membrane Nanopore	[43]	3	172	6	2366	66.3	5	6	1	0.25	1275	83.7	140	R
10	Single Staple Loop	[44]	2	195	6	2	100.0	1	6	0	0.05	2	100.0	4	=
11	DNA Frame	[45]	2	222	–	–	–	–	6	3	0.55	174	99.5	71	R
12	Rothemund Rectangle	[25]	2	226	–	–	–	–	6	3	0.25	126	100.0	65	R
13	Rectangle Variant	[46]	2	226	–	–	–	–	6	3	0.30	114	100.0	57	R
14	Small Moon	[47]	2	234	–	–	–	–	5	2	0.05	258	99.1	367	R
15	Rothemund Smiley	[25]	2	243	–	–	–	–	5	2	0.15	172	99.2	199	R
16	Rothemund Star	[25]	2	244	–	–	–	–	6	4	0.45	116	99.6	110	R
17	Capsule	[48]	3	264	–	–	–	–	–	–	–	–	–	–	–

					NAIVE Solver				REVNANO Solver						
ID	Wireframe Origami	Ref	Dim	Staples	$\mu_{\min}$	$d(\mathbf{g}, \mathbf{r})$	SP%	Wall(s)	$\mu_{\min}$	σ	β	$d(\mathbf{g}, \mathbf{r})$	SP%	Wall(s)	Vs.
18	Triangle	[37]	2	7	6	46	85.7	< 1	5	0	0.05	8	100.0	< 1	R
19	Square	[37]	2	8	6	6	100.0	< 1	6	0	0.05	6	100.0	< 1	=
20	Pentagon	[37]	2	10	6	6	100.0	< 1	6	0	0.05	6	100.0	< 1	=
2 1	Tetrahedron	[37]	3	13	5	141	76.9	< 1	5	0	0.05	4	100.0	< 1	R
2 2	Triangle Mesh	[37]	2	22	5	168	77.3	< 1	5	0	0.05	35	95.5	< 1	R
23	Cube	[37]	3	25	5	502	56.0	< 1	5	0	0.05	6	100.0	< 1	R
24	Star Mesh	[37]	2	38	6	443	76.3	< 1	5	0	0.05	66	97.4	1	R
25	Dodecahedron	[37]	3	59	–	–	–	–	5	0	0.10	188	96.6	3	R
26	Icosahedron	[37]	3	64	–	–	–	–	5	2	0.15	355	89.1	4	R
27	Square Mesh 1	[37]	2	82	–	–	–	–	5	4	0.05	284	92.7	78	R
28	Hexagon Mesh 1	[37]	2	84	–	–	–	–	5	2	0.25	335	92.9	13	R
29	Annulus Mesh 1	[37]	2	89	–	–	–	–	5	0	0.05	91	98.9	7	R
30	Hexagonal Tile	[37]	2	98	–	–	–	–	5	0	0.05	169	98.0	12	R
31	Truncated Cube	[37]	3	98	–	–	–	–	6	2	0.05	72	100.0	6	R
32	Cross Mesh	[37]	2	110	–	–	–	–	5	1	0.15	176	97.3	18	R
33	vHelix Ball	[49]	3	132	6	115	98.5	1	6	0	0.20	18	100.0	5	R
34	Annulus Mesh 2	[37]	2	161	–	–	–	–	5	3	0.05	106	100.0	131	R
35	Lotus Mesh	[37]	2	180	–	–	–	–	5	3	0.05	271	97.8	255	R
36	Enneagonal Trapezohedron	[37]	3	318	–	–	–	–	–	–	–	–	–	–	–

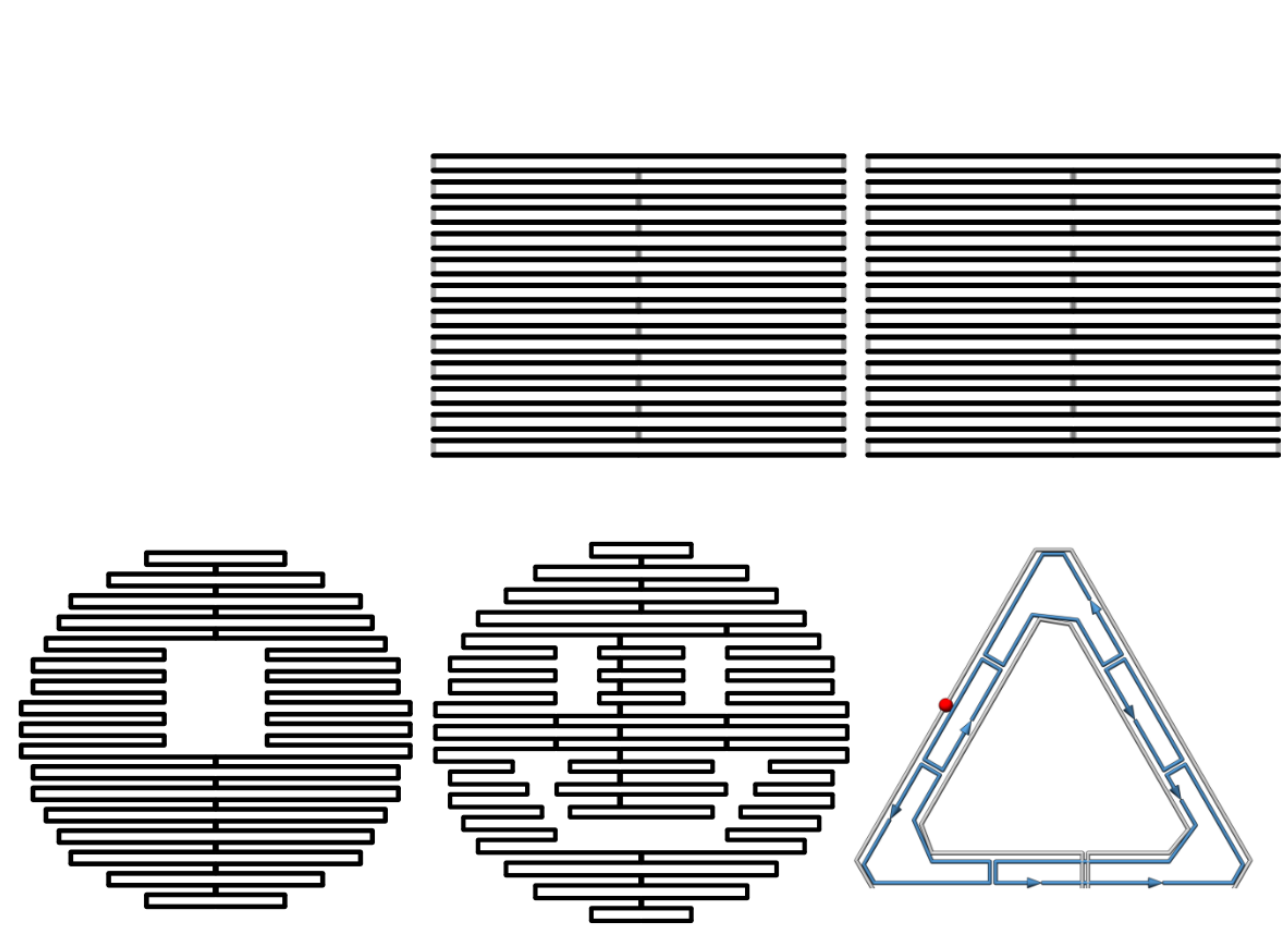
Results

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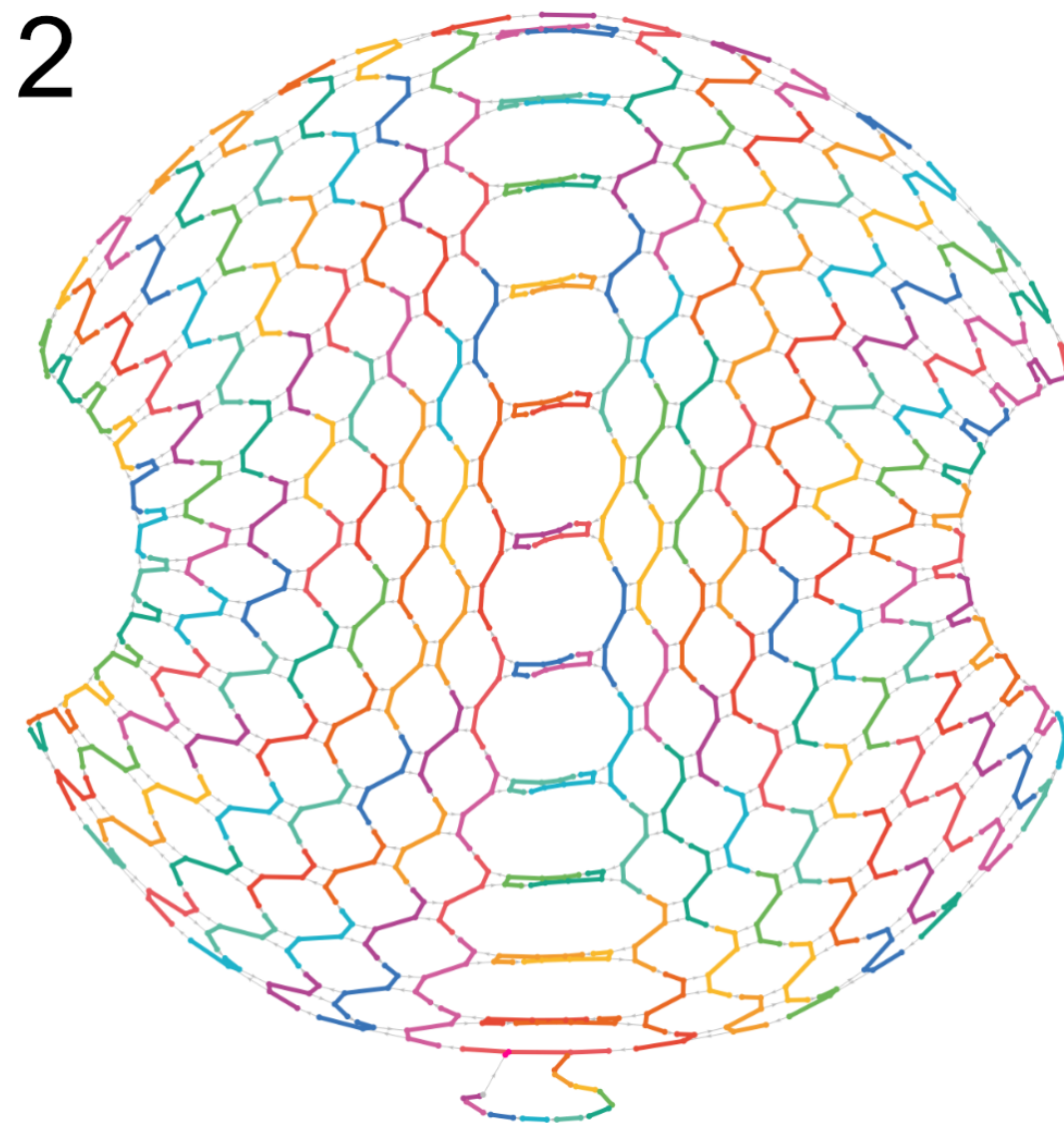


Results

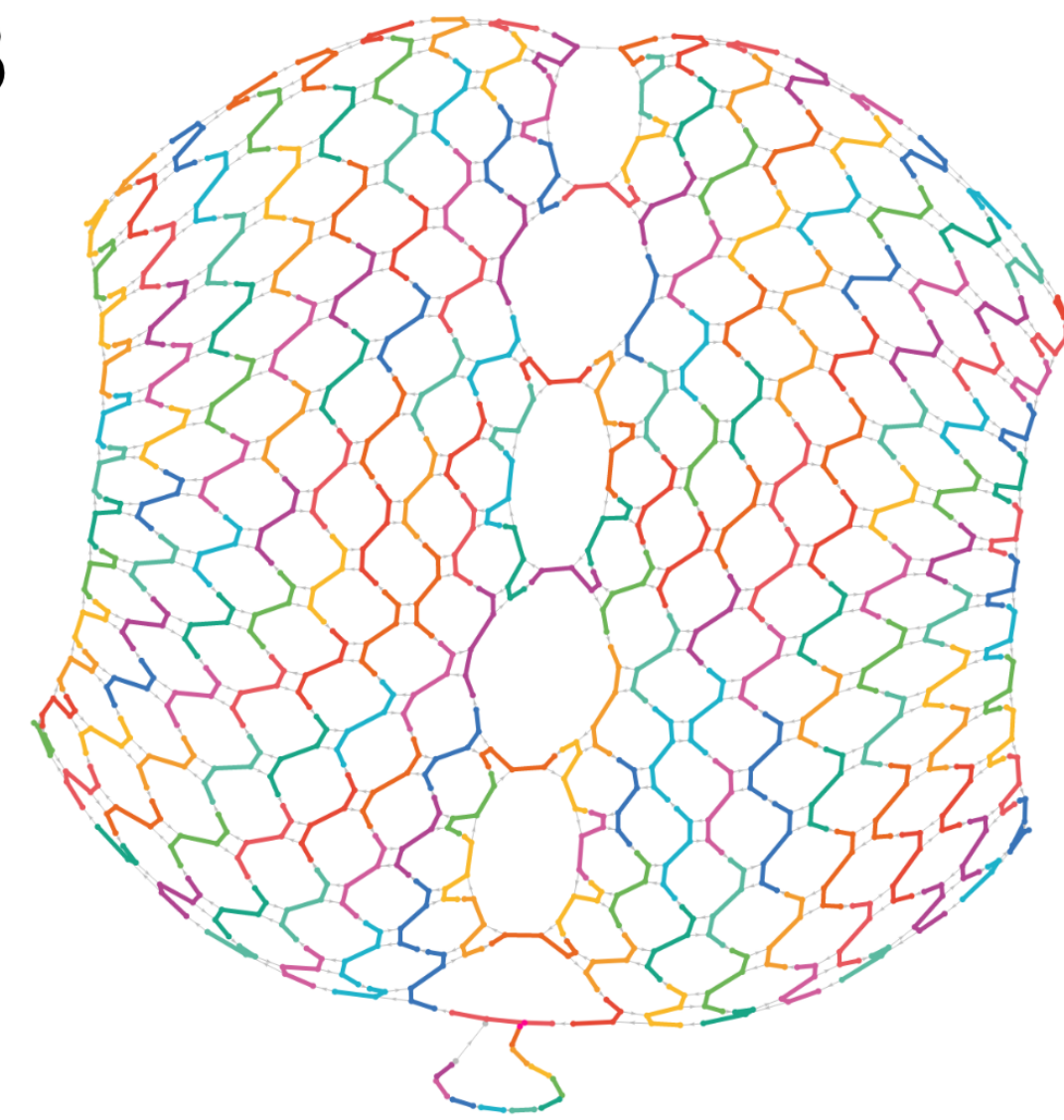
revnano.readthedocs.io



12

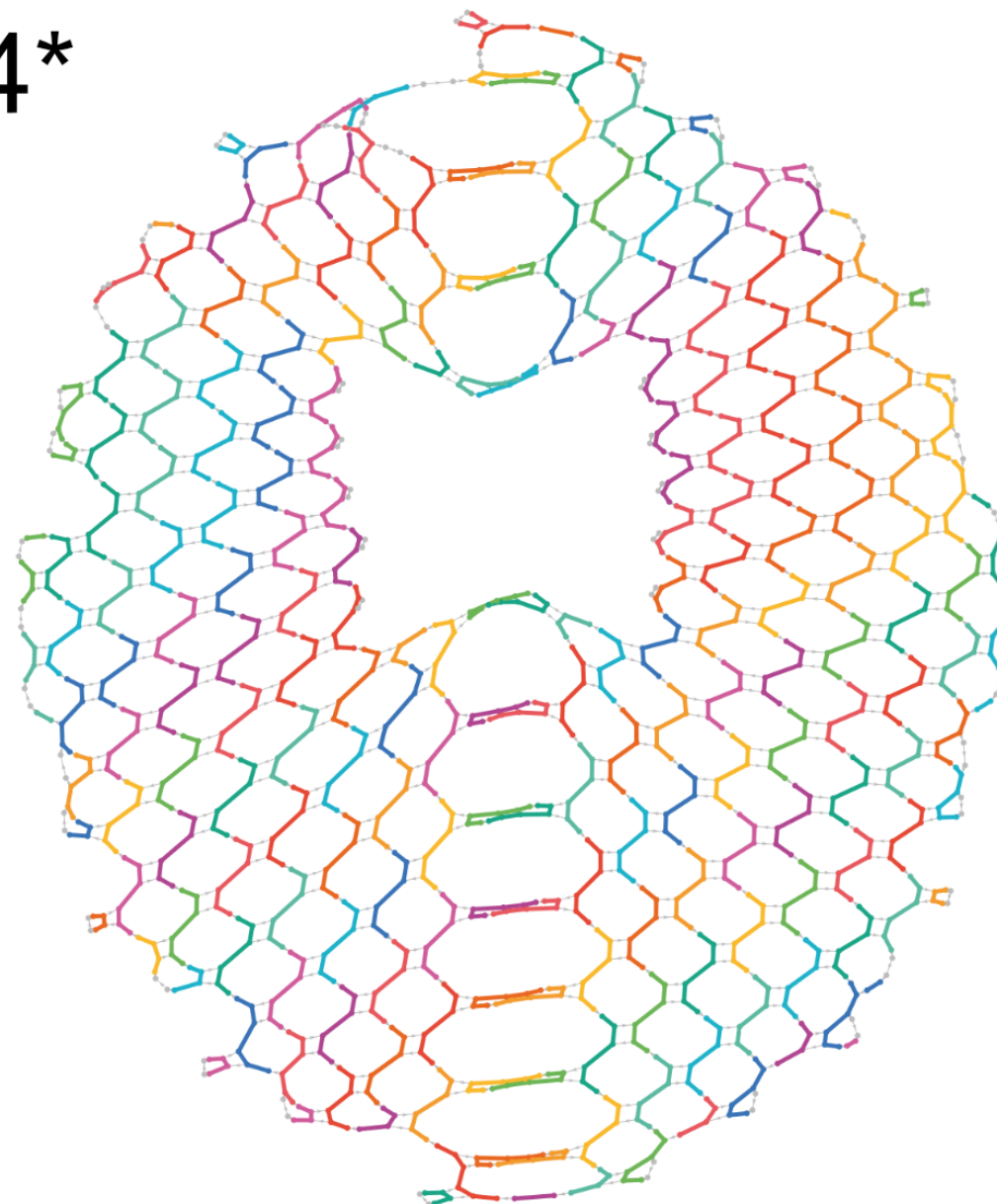


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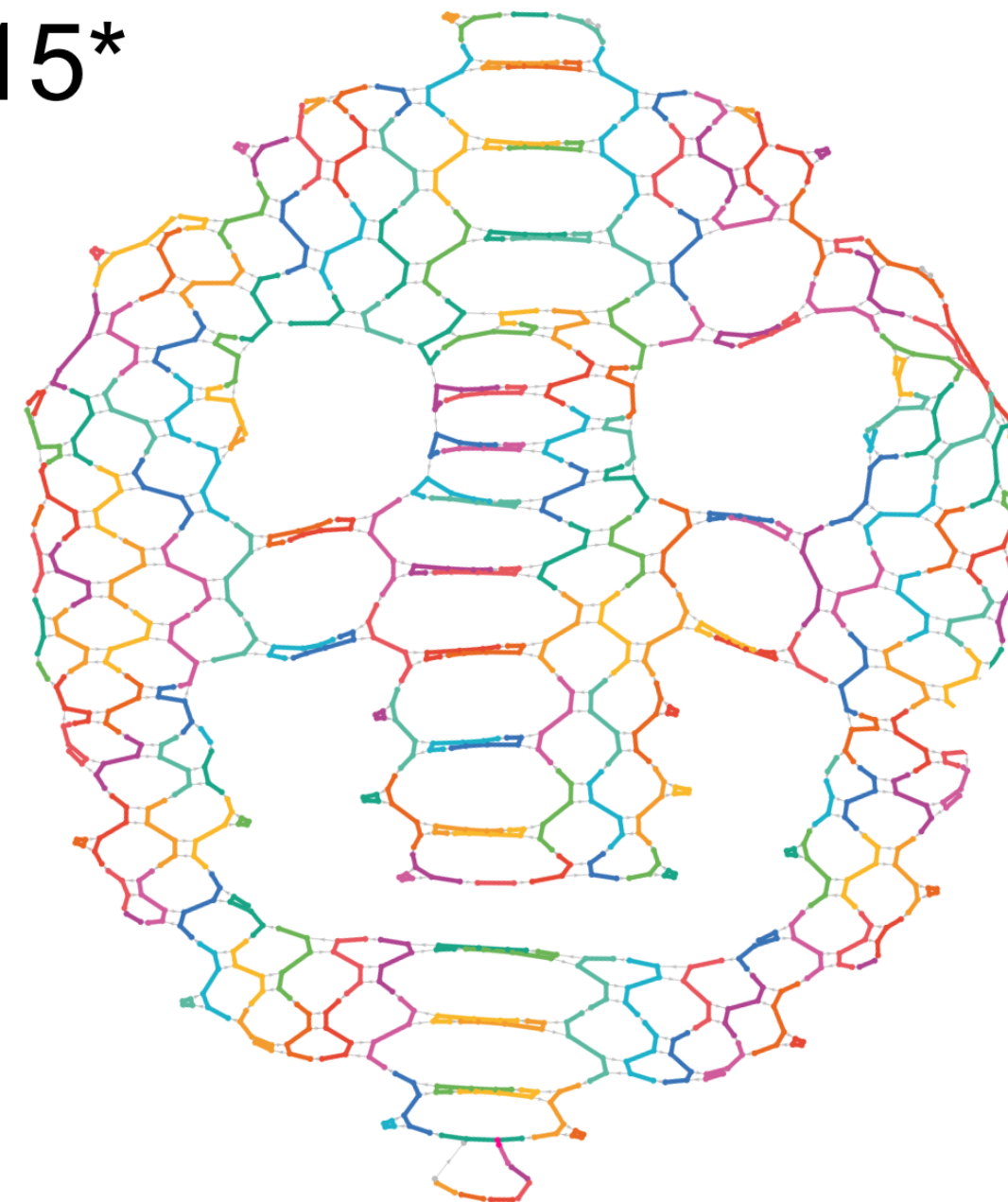


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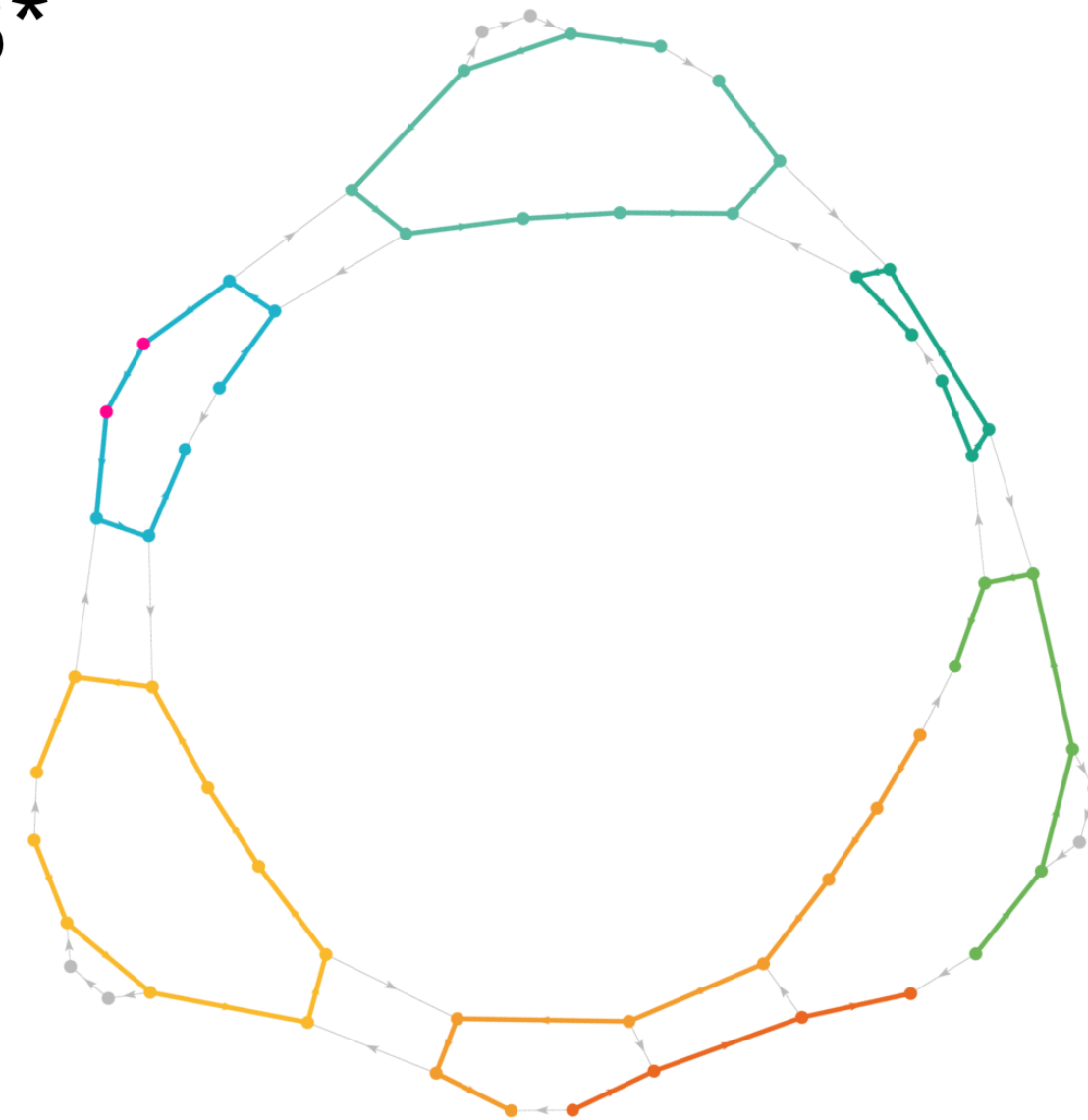
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15*

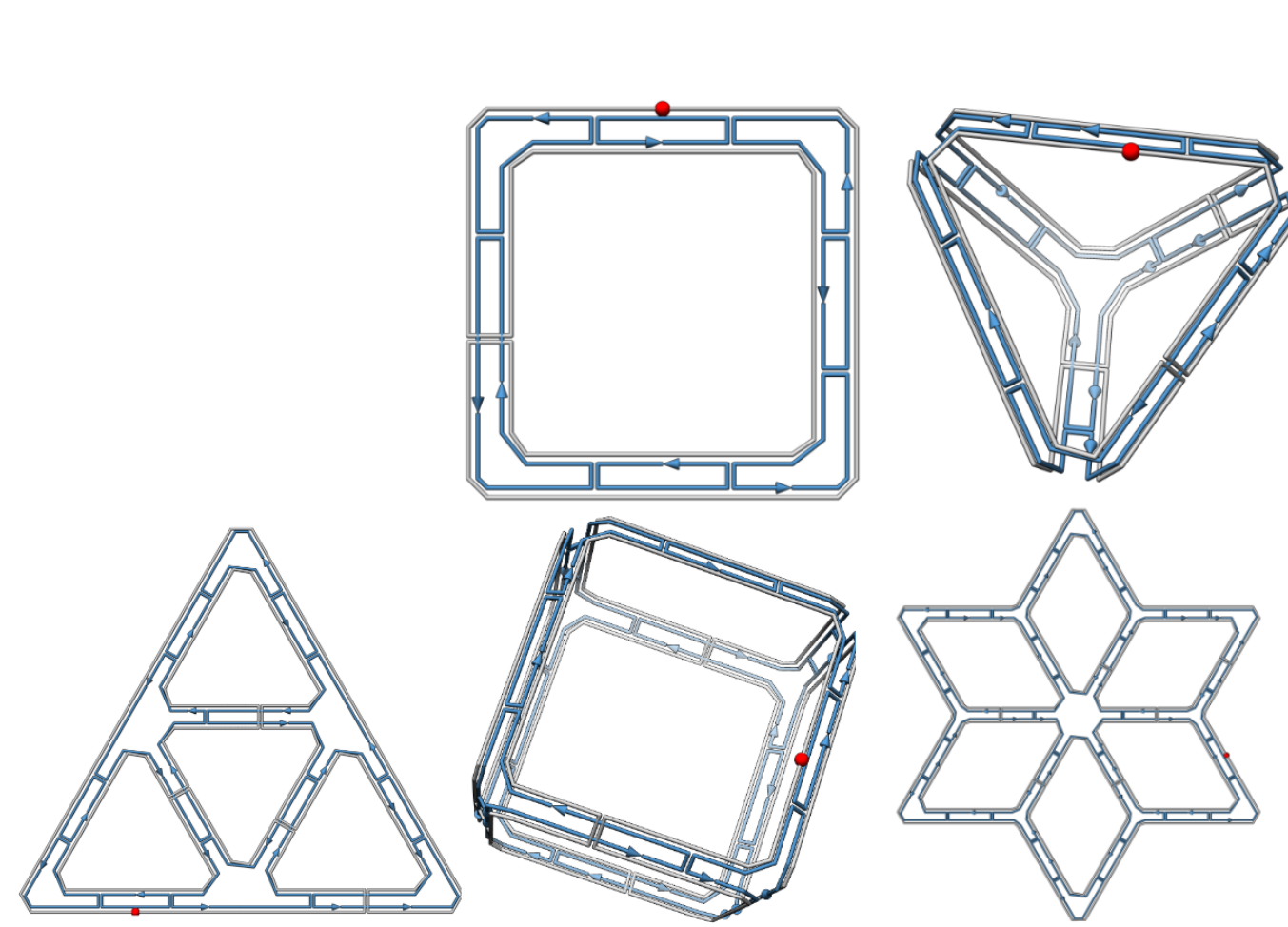


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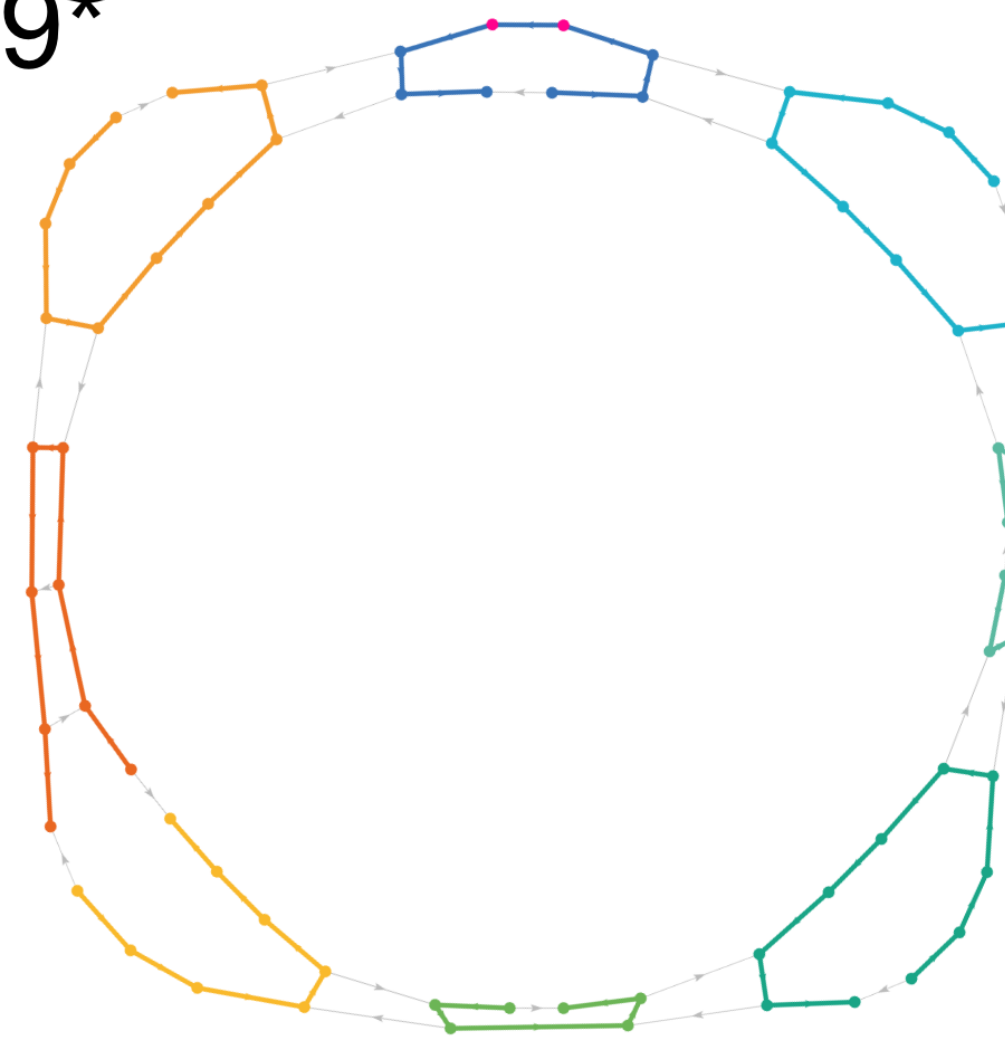


Results

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19*

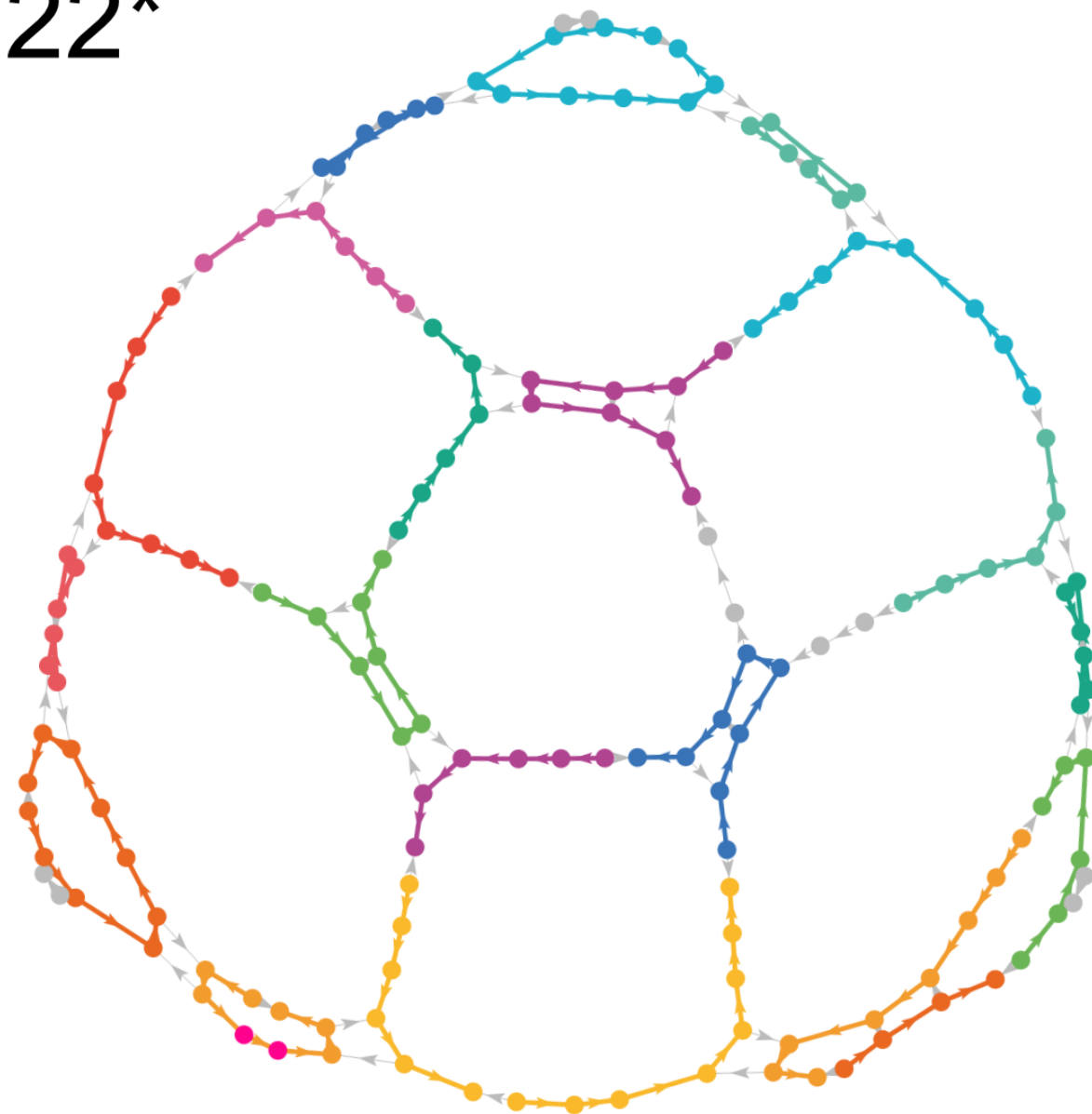


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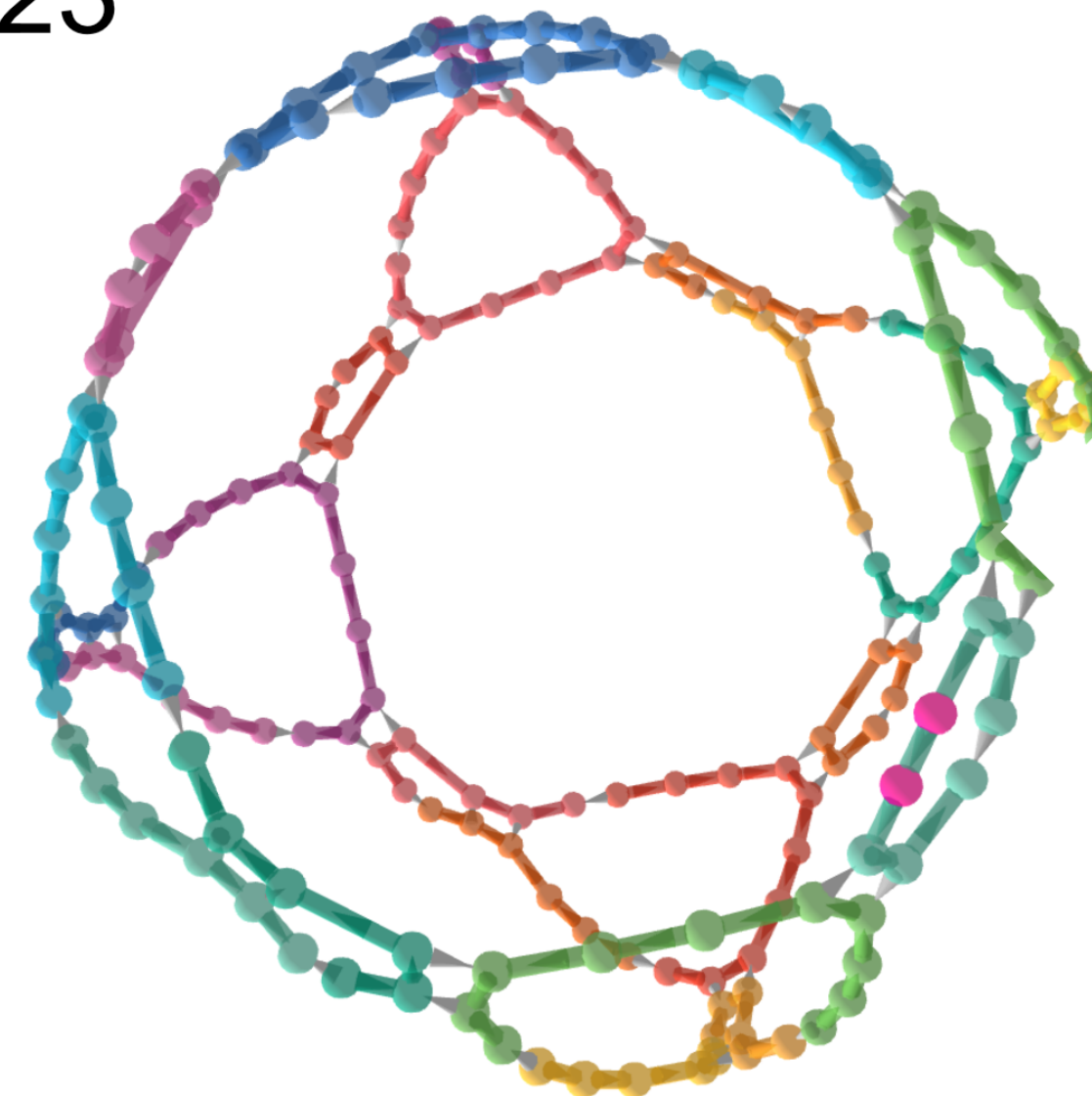


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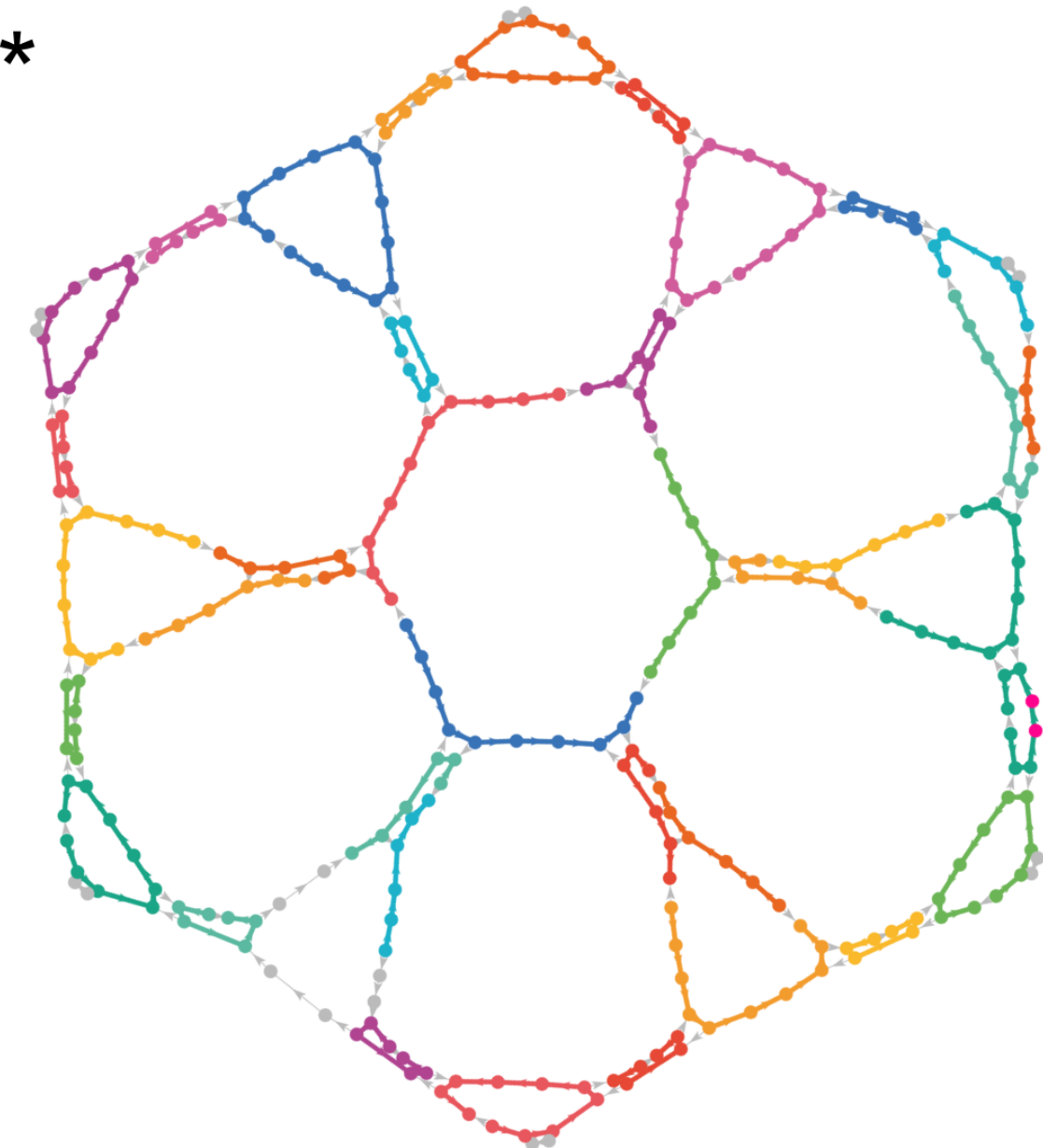
22*



23



24*



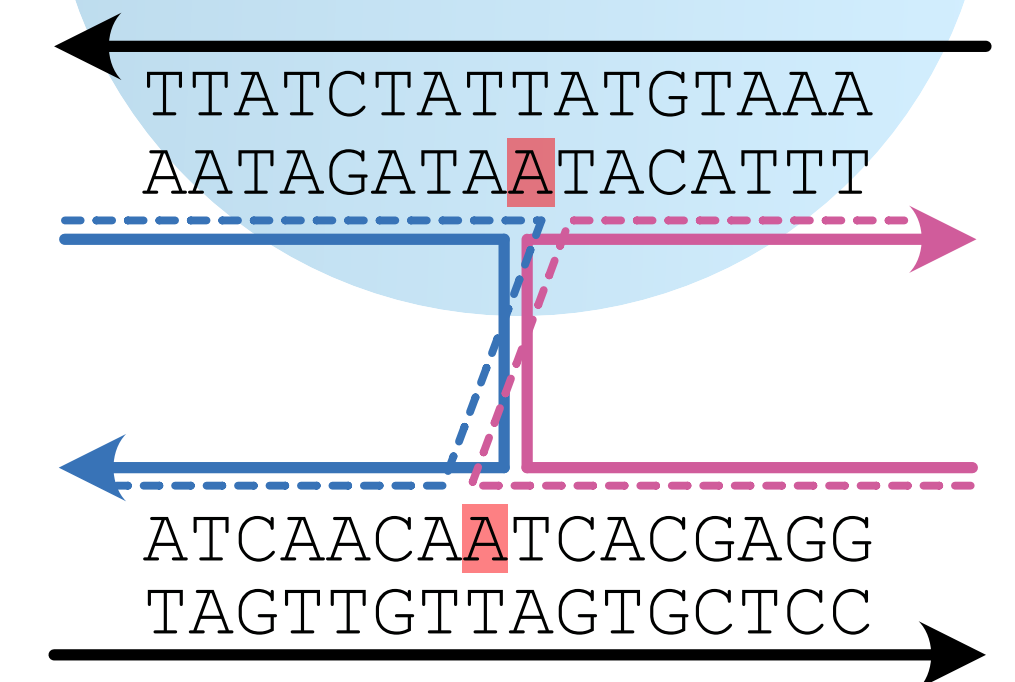
Some Limitations / Challenges

Parameter
dependence

$(\mu_{\min}, \sigma, \beta)$

Short (e.g. 5nt or
less) hybridising
staple sections
problematic

Sliding holliday
junctions provide
ambiguity

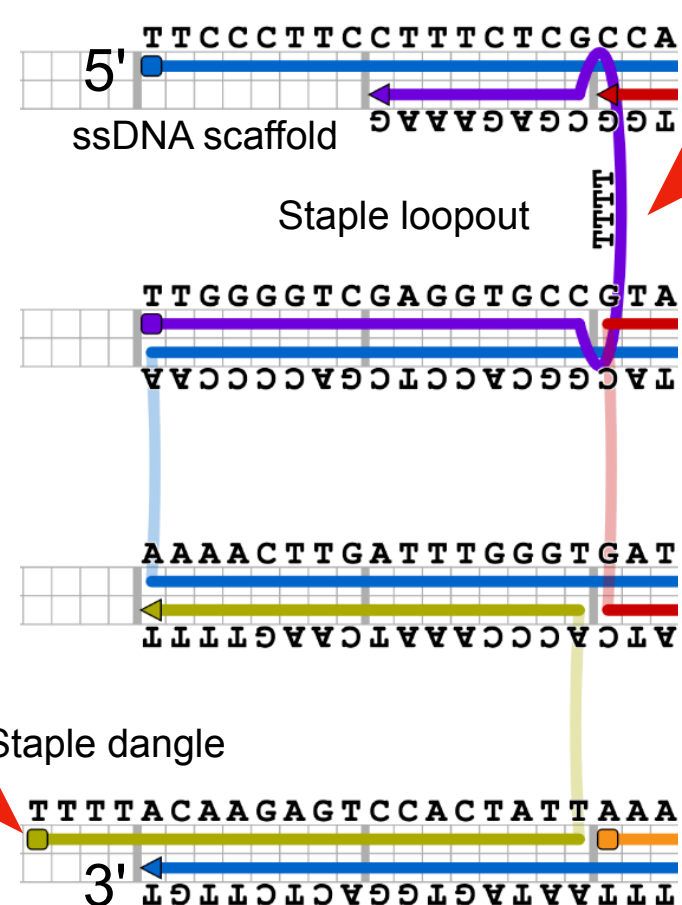


Staple
misplacement is
quite hard to
detect

Guide
Schematic is
not editable

3D raster
shapes are
dense and
hard to
decipher

Staple dangling
ends and interior
loopouts need
marking



Other Interesting Possibilities

Encode the
contact map for
an origami within
it's sequences

Convert Guide
Schematic to
oxDNA format
for relaxation

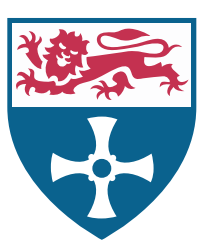
Underpin ML
applications in
structural DNA
nanotech



Royal Academy
of Engineering



Engineering and
Physical Sciences
Research Council



Newcastle
University

Jordan Connolly

Juan Elezgaray

Emanuela Torelli

Silvia Navarro

Jaume Barcardit

Prof. Natalio Krasnogor

**Many thanks for the
invitation to speak at
DNA Nanotech in Action !**