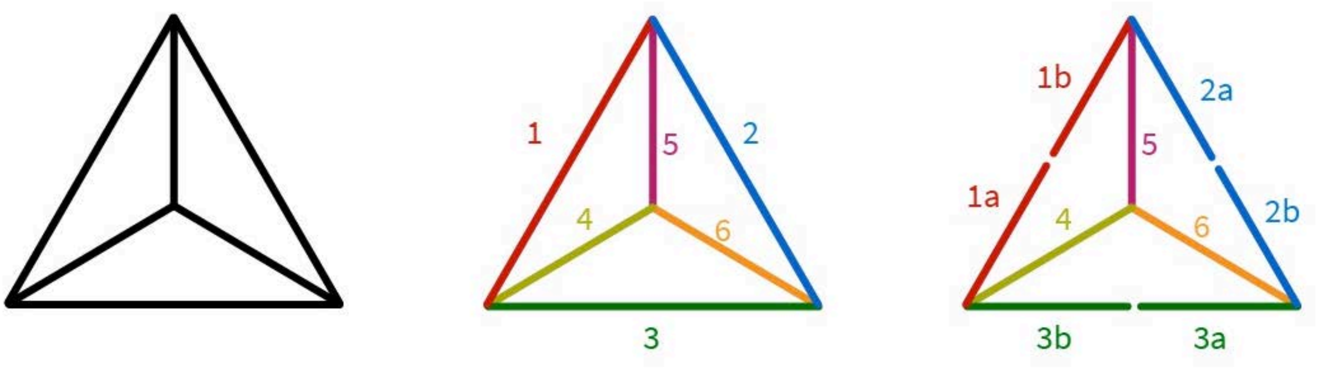
Design 3: Wireframe Tetrahedron

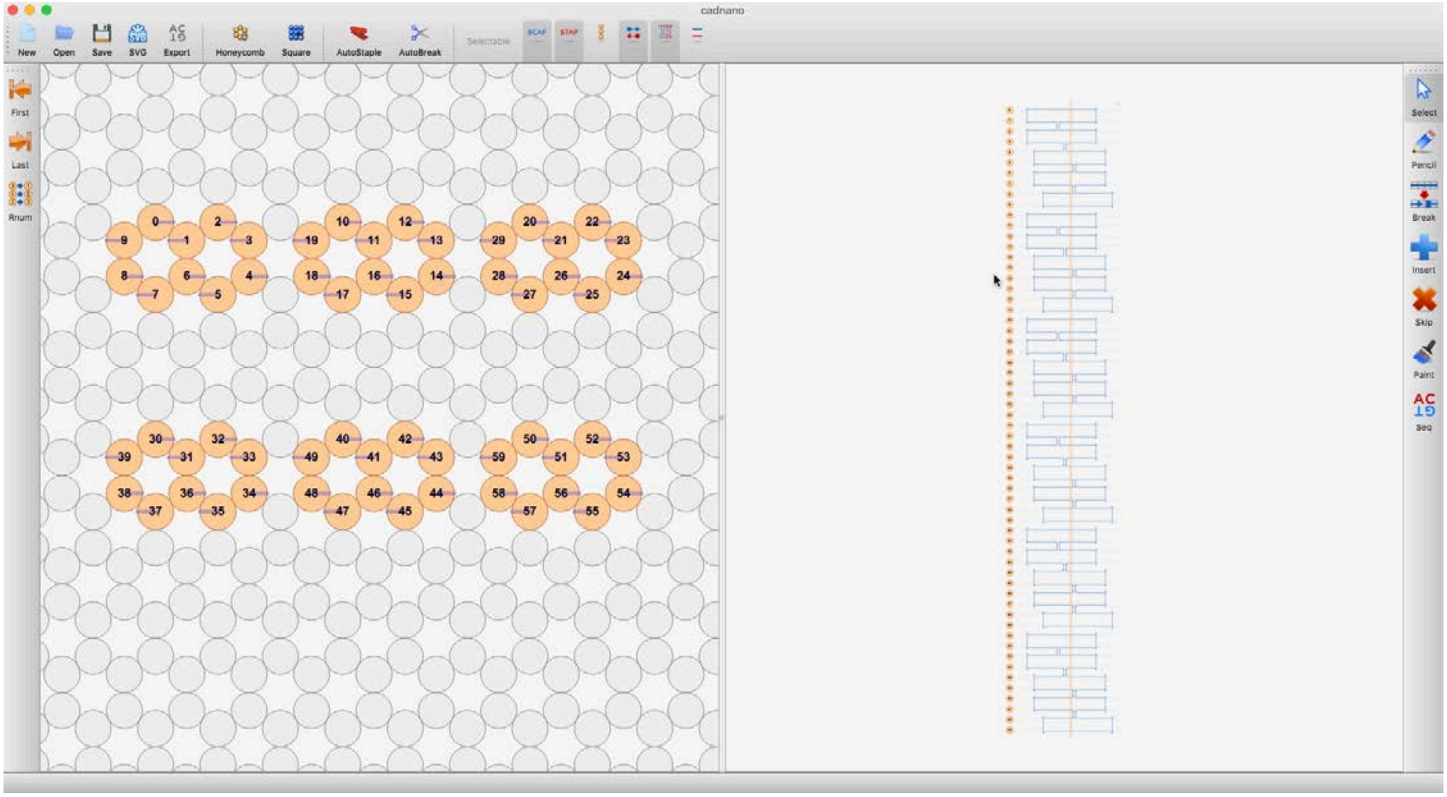
Step 1: Starting with a Schlegel diagram, decide which edges are going to be split to avoid any closed loops in the graph.

This diagram is drawn manually in Illustrator.



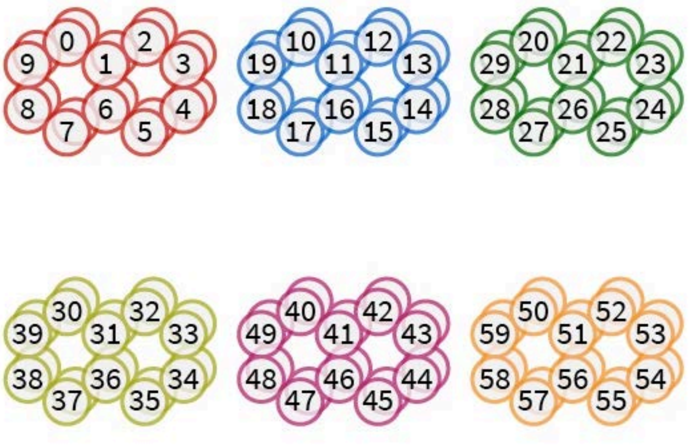
Step 2: Create strut cross-sections in Cadnano

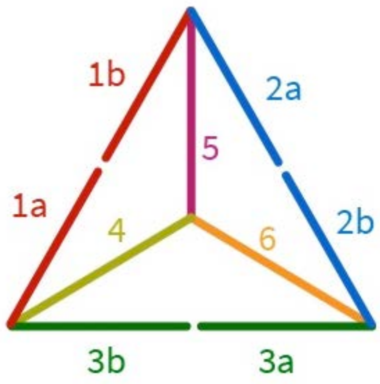
We use six 10-helix bundles. Once the basic cross-section is defined, use **Cadnano1** to export the SVG diagram. (Cadnano2 SVG doesn't provide the cross-section, but we are working on a new SVG exporter as part of CTK).



Step 3: Import the SVG and stylize the Virtual Helices.

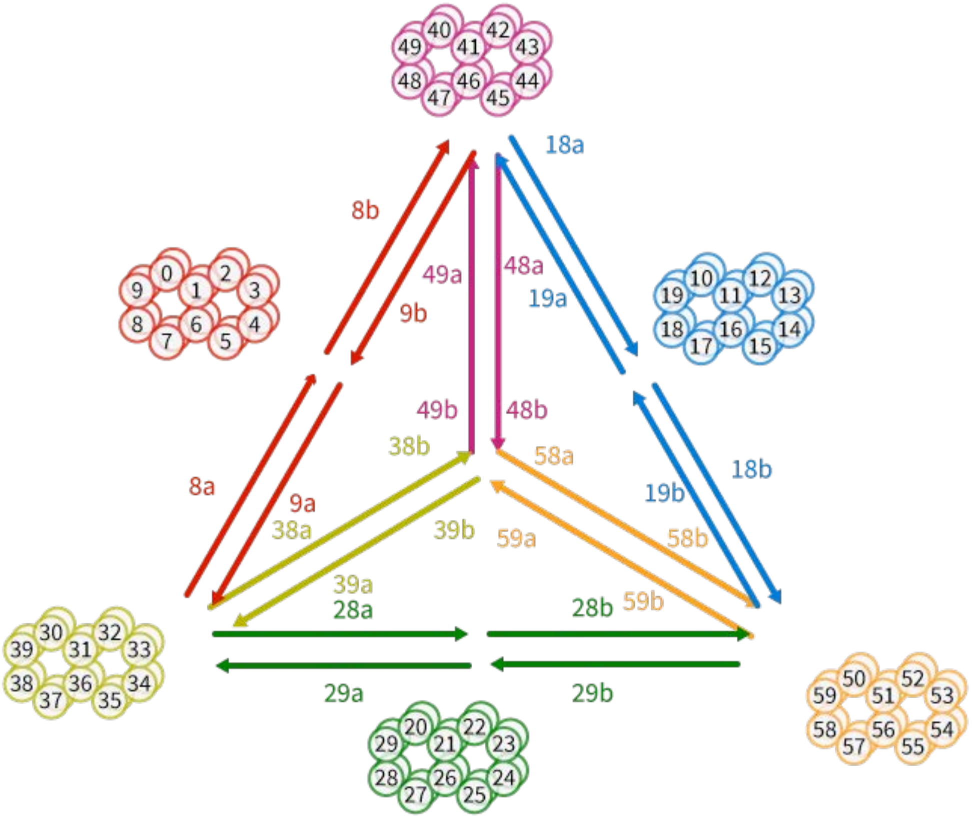
Assign colors to the different struts to match the Schlegel diagram. You can duplicate the circles and apply a white fill with some transparency to the front circles to get a “pseudo 3D” effect.





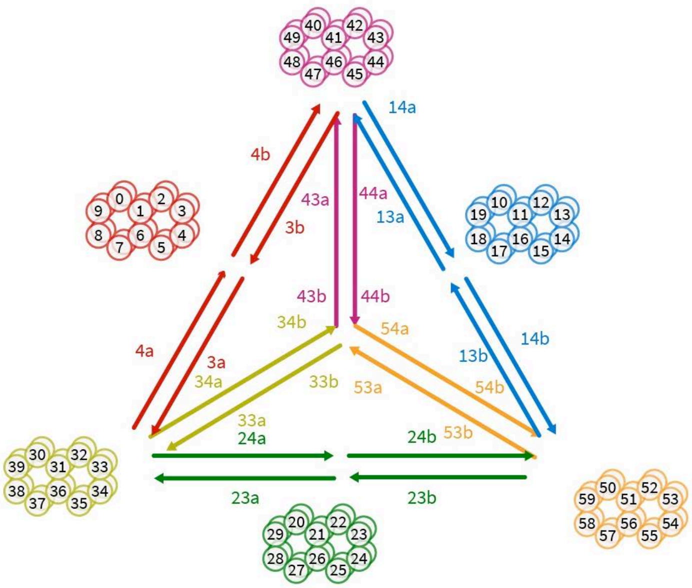
Step 4: Re-draw the Schlegel diagram

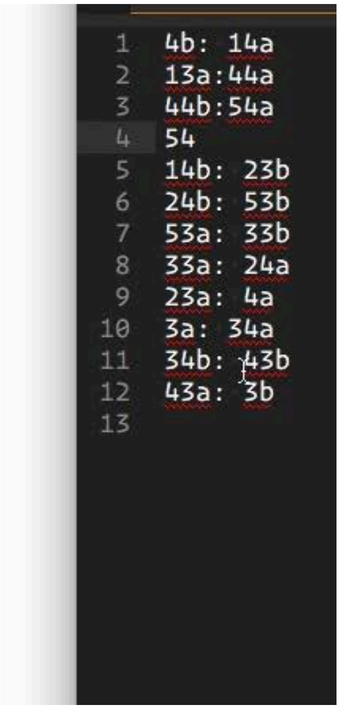
Double the lines to include“fwd” and “rev” paths to correspond to “even” and “odd” helices in our design. Number the edge segments to match the helix numbers for the corresponding strut. Add arrows to indicate 3’ ends.



Step 5: Trace a complete path through the segments and note connection pairs

Working clockwise starting at segment **4b**, it connects to **14a**, which crosses over to **13a**, which connects to **44a**, and so on. We keep track of these pairings in a text editor.

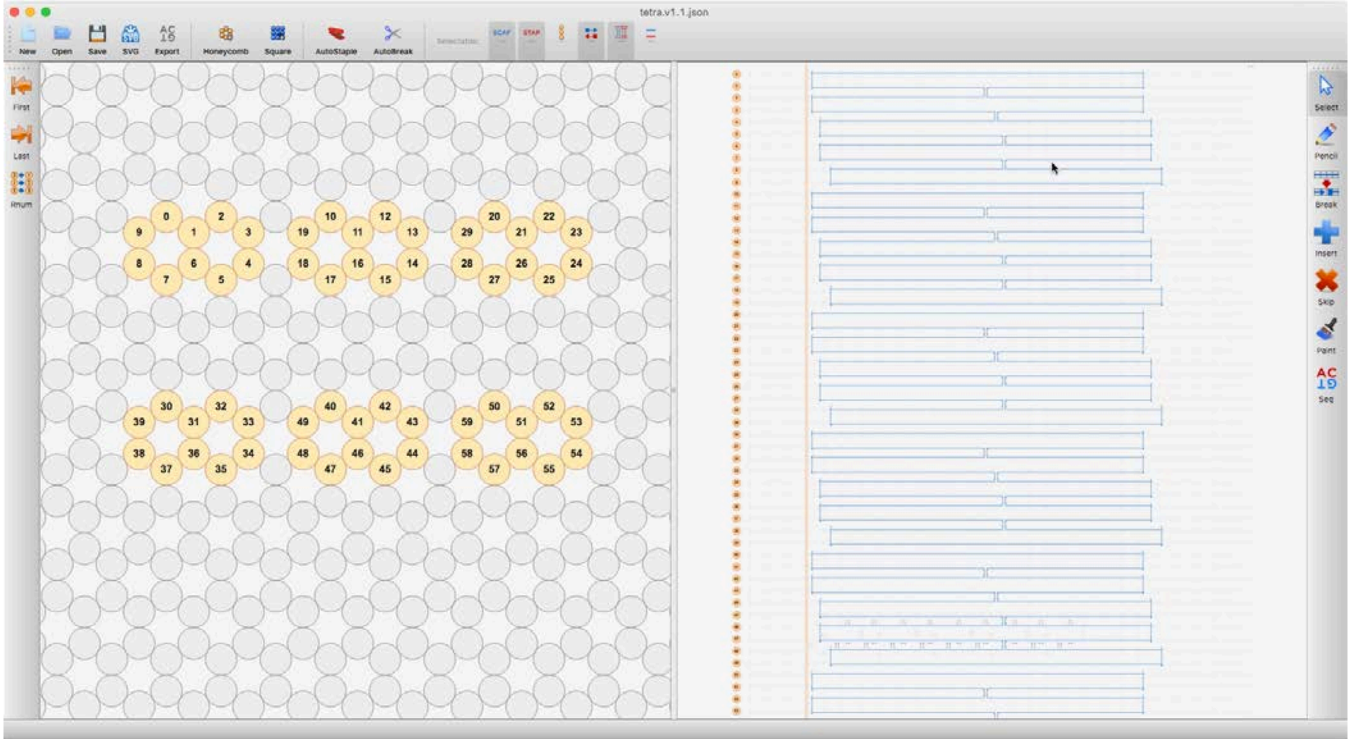




```
4b: 14a
13a:44a
44b:54a
54
14b: 23b
24b: 53b
53a: 33b
33a: 24a
23a: 4a
3a: 34a
34b: 43b
43a: 3b

```

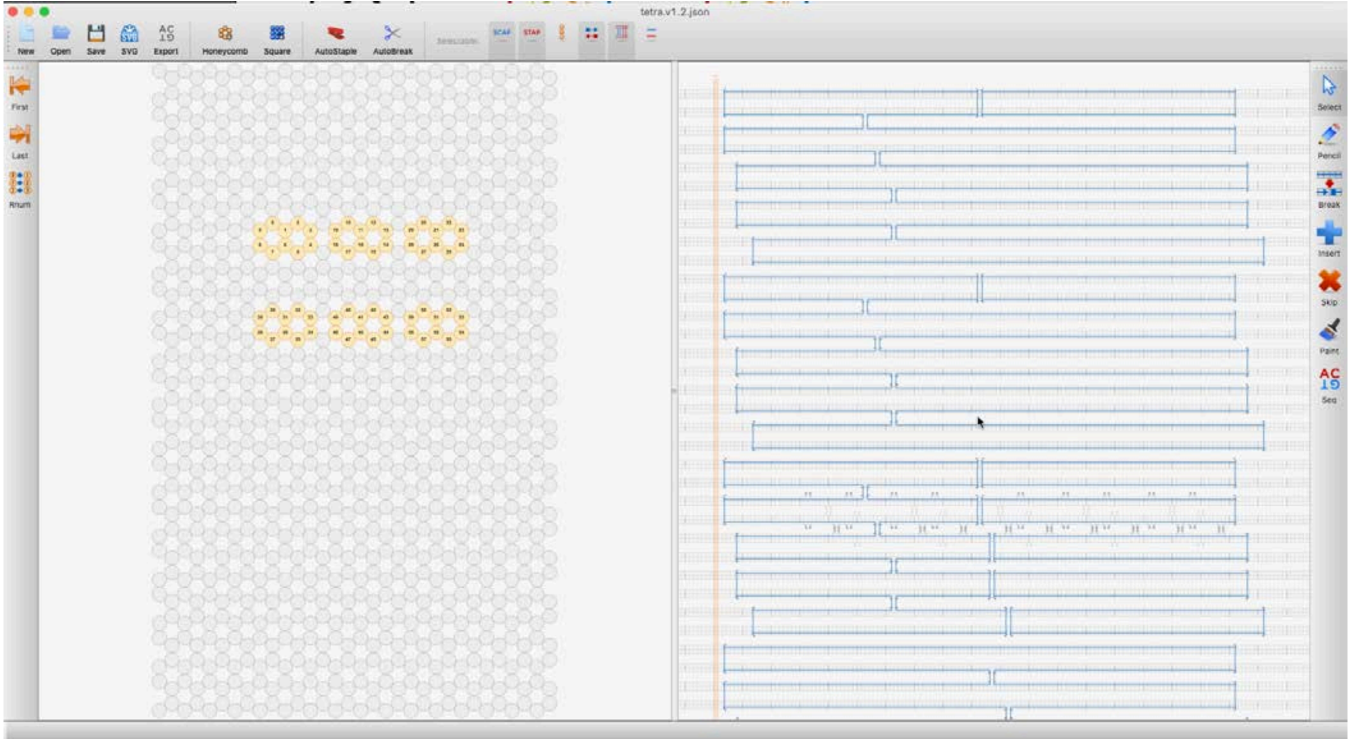
Step 6: Return to the Cadnano design and extrude the struts to desired lengths

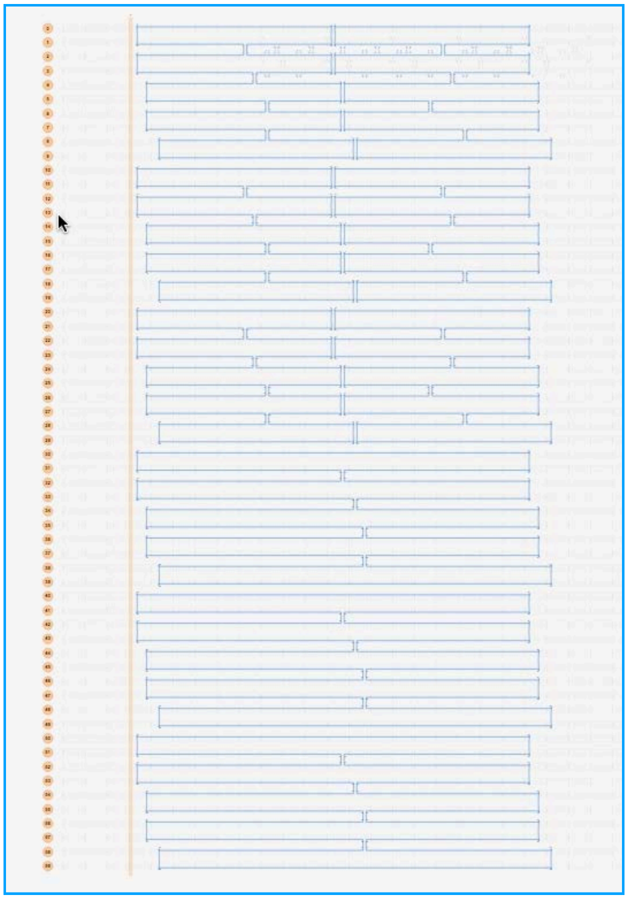
Make sure the sum of the lengths matches the desired scaffold length, e.g. 6 x 1344 = **8064**



Step 7: Install Scaffold crossovers to split the appropriate struts in half.

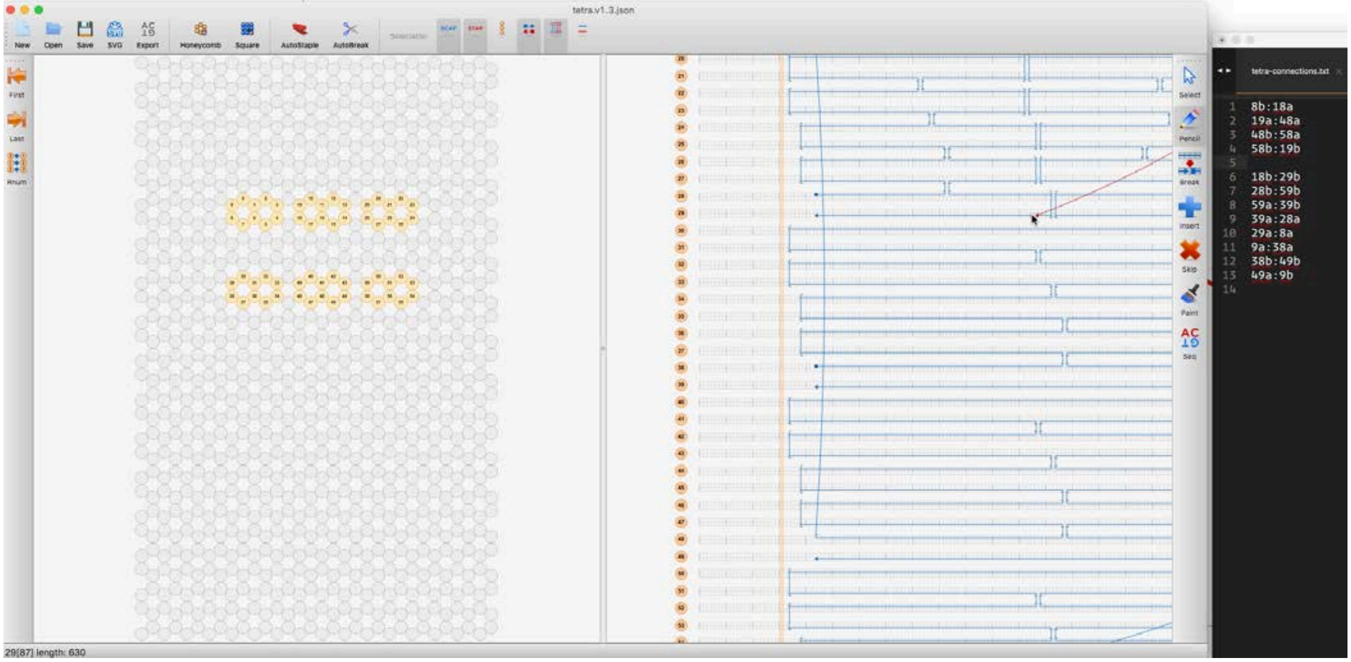
We must also install new seams in the half-struts to avoid any disconnected segments.





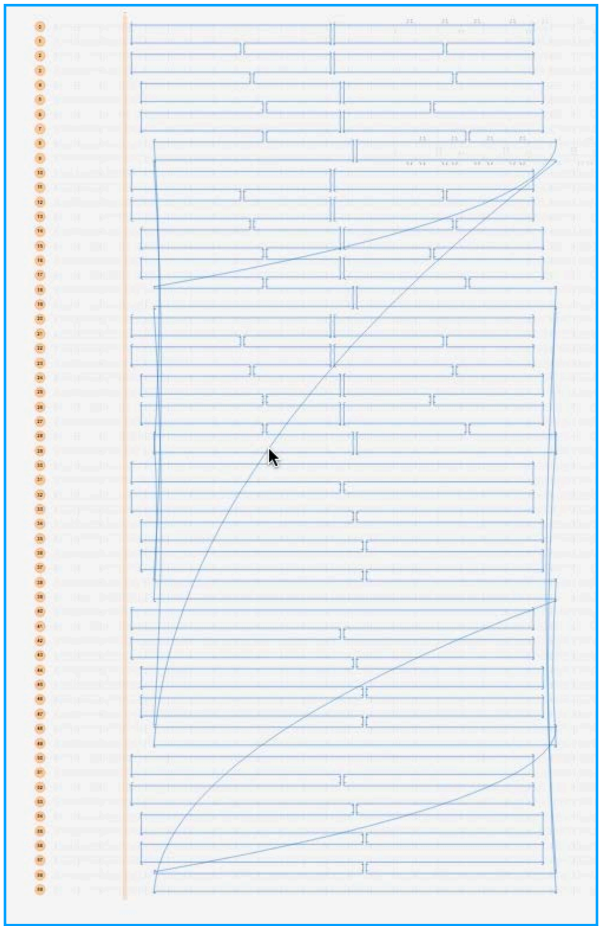
The updated scaffold layout.

Step 8: Use the Pencil tool to force-install the vertex connections in the scaffold.



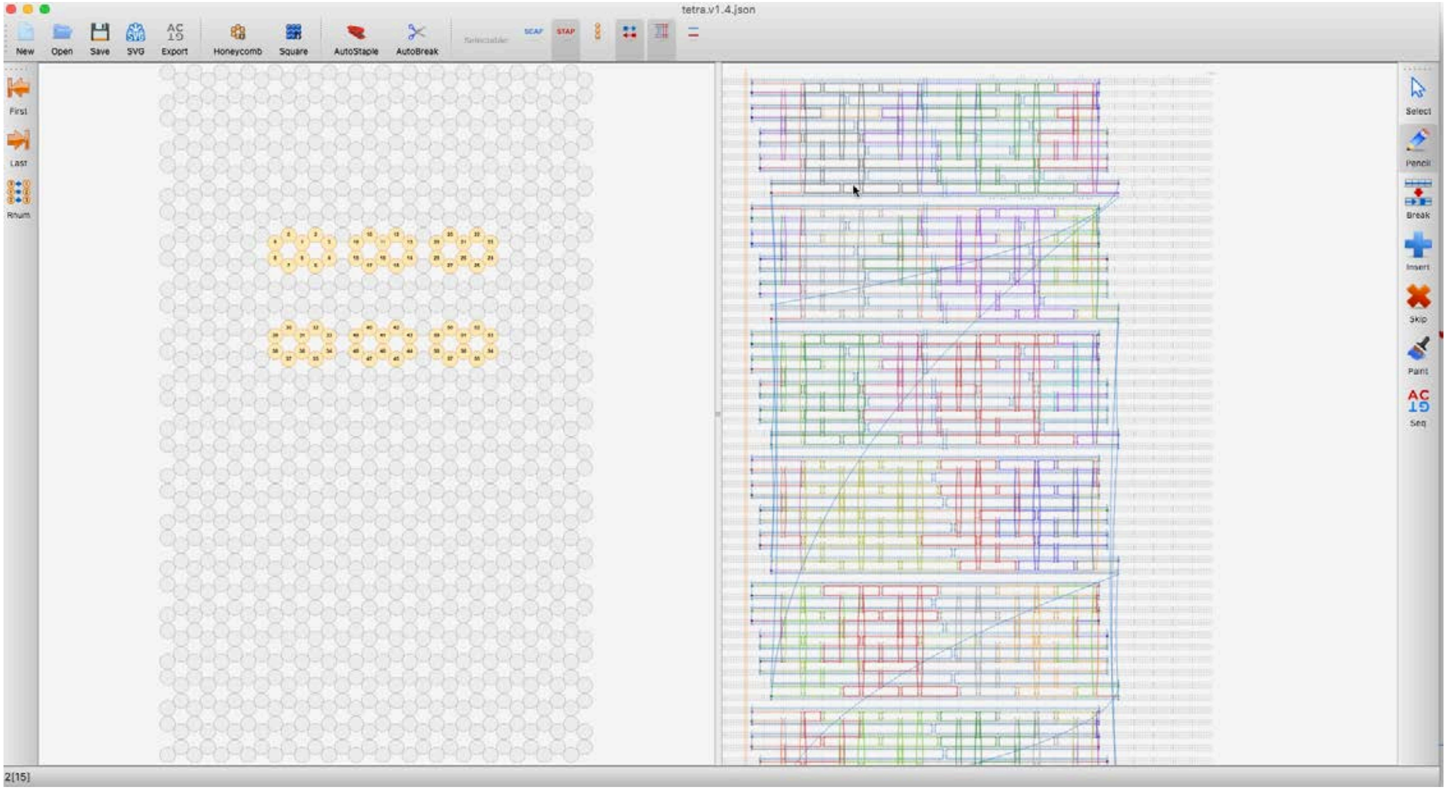
```
8b:18a
19a:48a
48b:58a
58b:19b

18b:29b
28b:59b
59a:39b
39a:28a
29a:8a
9a:38a
38b:49b
49a:9b
```

29[87] length: 630

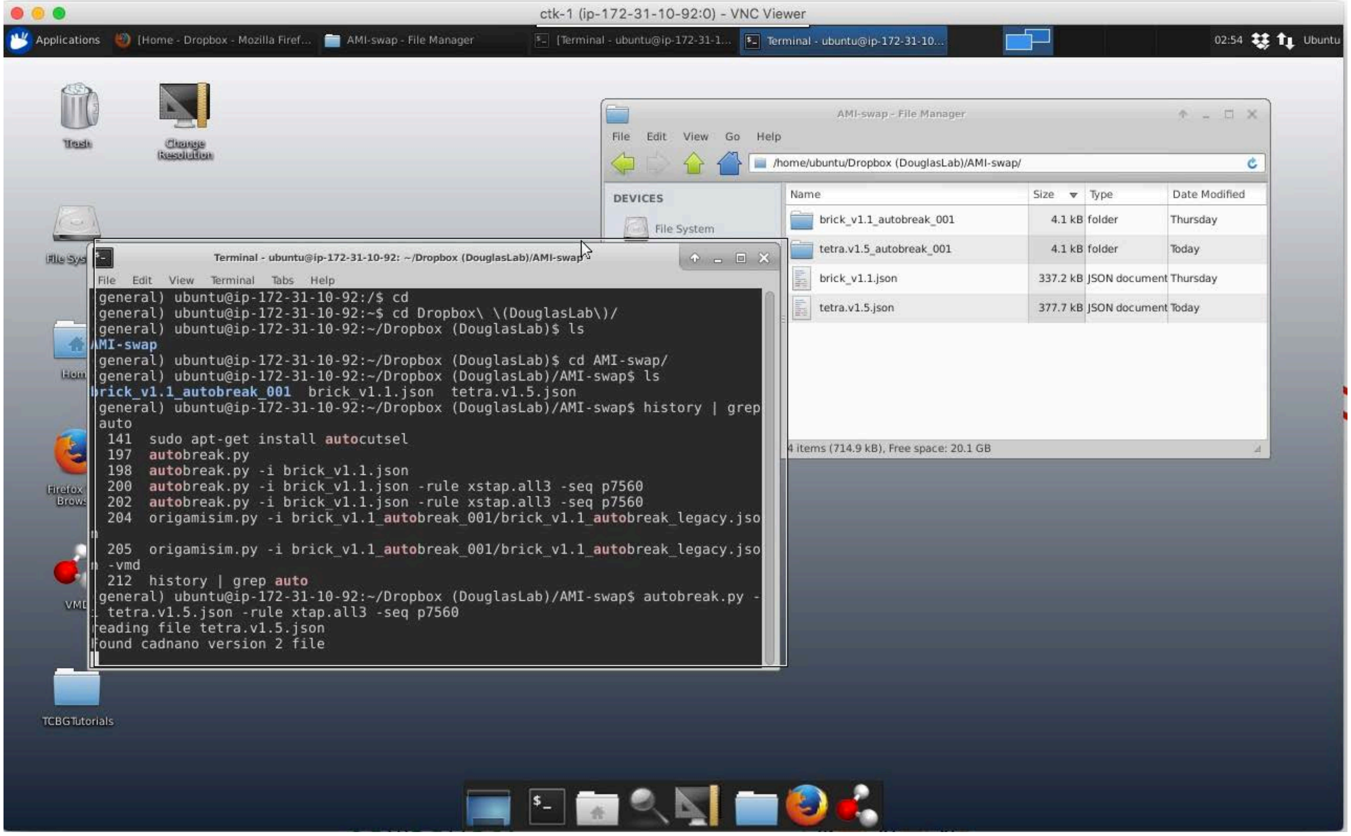


The final scaffold layout.

Step 9: Use AutoStaple to create proto-staple paths. Clean up edges as usual.



Step 10: Transfer design to the AMI and run AutoBreak


ctk-1 (ip-172-31-10-92:0) - VNC Viewer
Applications
[Home - Dropbox - Mozilla Firef...
AMI-swap - File Manager
[Terminal - ubuntu@ip-172-31-1...
Terminal - ubuntu@ip-172-31-10...
02:54
Ubuntu
Trash
Change Resolution
File Sys
Hom
Firefox Brow
VMD
TCBGTutorials
AMI-swap - File Manager
File
Edit
View
Go
Help
DEVICES
File System
Terminal - ubuntu@ip-172-31-10-92: ~/Dropbox (DouglasLab)/AMI-swap
File
Edit
View
Terminal
Tabs
Help

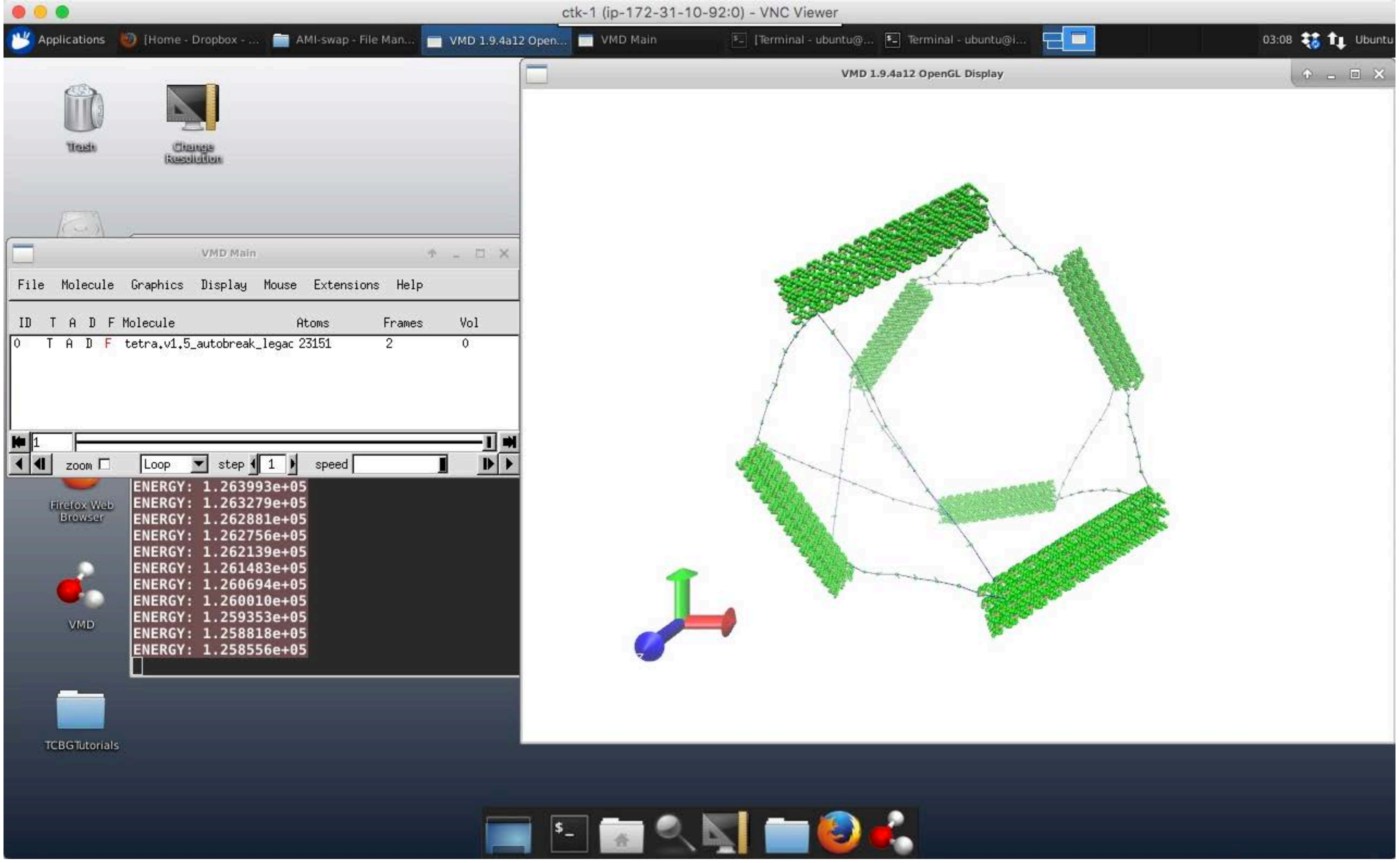
/home/ubuntu/Dropbox (DouglasLab)/AMI-swap/

Name	Size	Type	Date Modified
brick_v1.1_autobreak_001	4.1 kB	folder	Thursday
tetra.v1.5_autobreak_001	4.1 kB	folder	Today
brick_v1.1.json	337.2 kB	JSON document	Thursday
tetra.v1.5.json	377.7 kB	JSON document	Today

4 items (714.9 kB), Free space: 20.1 GB

```
general) ubuntu@ip-172-31-10-92:/$ cd
general) ubuntu@ip-172-31-10-92:~$ cd Dropbox\ \(DouglasLab\)/
general) ubuntu@ip-172-31-10-92:~/Dropbox (DouglasLab)$ ls
AMI-swap
general) ubuntu@ip-172-31-10-92:~/Dropbox (DouglasLab)$ cd AMI-swap/
general) ubuntu@ip-172-31-10-92:~/Dropbox (DouglasLab)/AMI-swap$ ls
brick_v1.1_autobreak_001  brick_v1.1.json  tetra.v1.5.json
general) ubuntu@ip-172-31-10-92:~/Dropbox (DouglasLab)/AMI-swap$ history | grep
auto
 141  sudo apt-get install autocutsel
 197  autobreak.py
 198  autobreak.py -i brick_v1.1.json
 200  autobreak.py -i brick_v1.1.json -rule xstap.all3 -seq p7560
 202  autobreak.py -i brick_v1.1.json -rule xstap.all3 -seq p7560
 204  origamisim.py -i brick_v1.1_autobreak_001/brick_v1.1_autobreak_legacy.jso
n
 205  origamisim.py -i brick_v1.1_autobreak_001/brick_v1.1_autobreak_legacy.jso
n -vmd
 212  history | grep auto
general) ubuntu@ip-172-31-10-92:~/Dropbox (DouglasLab)/AMI-swap$ autobreak.py -
i tetra.v1.5.json -rule xtap.all3 -seq p7560
reading file tetra.v1.5.json
found cadnano version 2 file
```

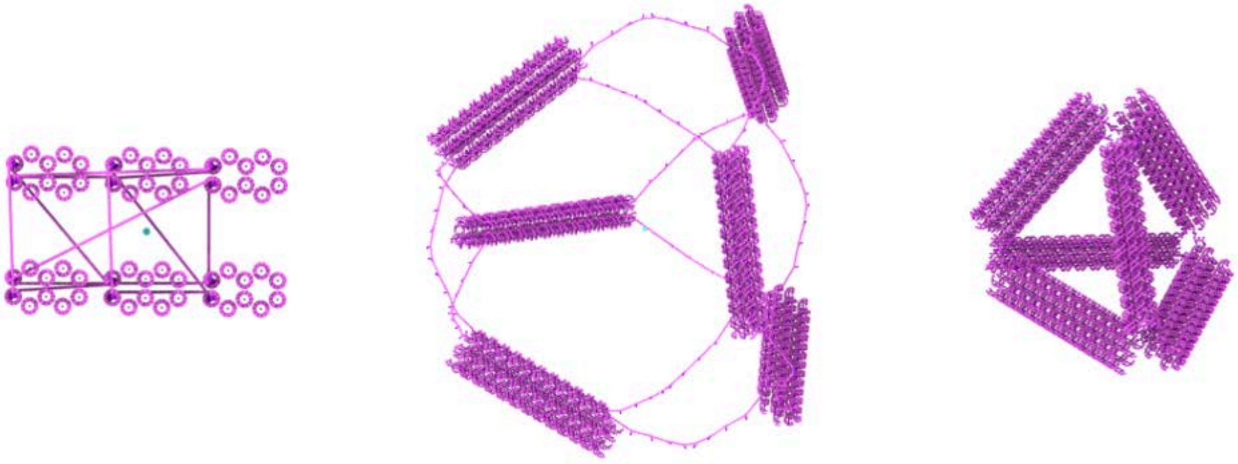
Step 11: Run OrigamiSim



```
ID  T  A  D  F Molecule                    Atoms   Frames   Vol
0   T  A  D  F  tetra.v1.5_autobreak_legac 23151   2        0
```

```
ENERGY:  1.263993e+05
ENERGY:  1.263279e+05
ENERGY:  1.262881e+05
ENERGY:  1.262756e+05
ENERGY:  1.262139e+05
ENERGY:  1.261483e+05
ENERGY:  1.260694e+05
ENERGY:  1.260010e+05
ENERGY:  1.259353e+05
ENERGY:  1.258818e+05
ENERGY:  1.258556e+05
```

Assuming you are working in your Dropbox swap folder, you should be able to open the **.gsd** files in **Ovito**.



Frame 0 Frame 9 Frame 32

Example Ovito renders of frames 0, 9, and 32 of the tetra.v1 simulation