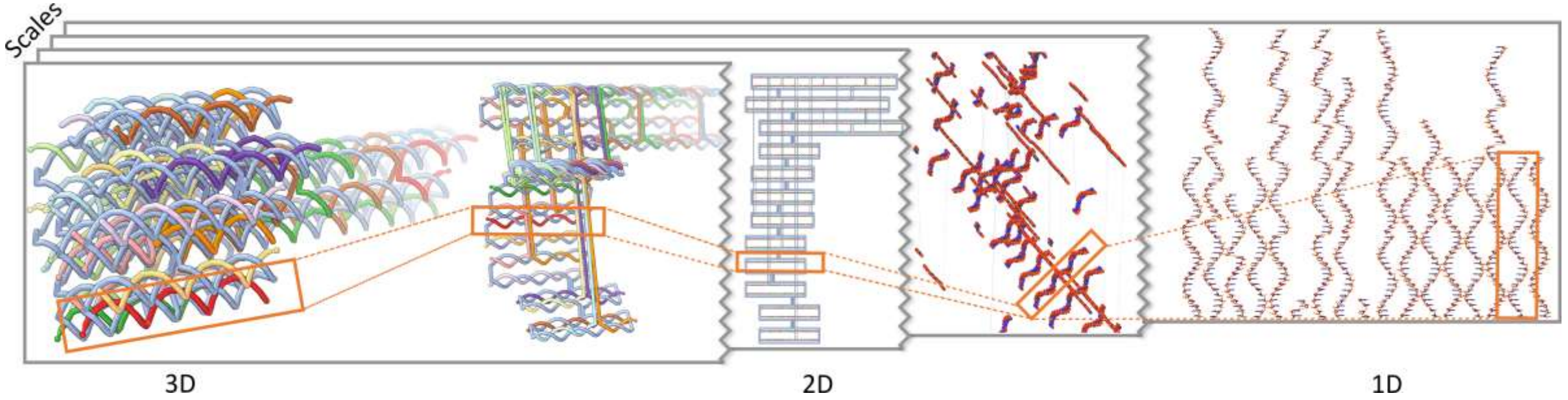
# DimSUM: Dimension and Scale Unifying Map for Visual Abstraction of DNA Origami Structures




H. Miao[1,2], E. D. Llano[2], T. Isenberg[3,4], M. E. Gröller[1,5], I. Barišić[2], I. Viola[1]

1 TECHNISCHE UNIVERSITÄT WIEN Vienna University of Technology

2 AUSTRIAN INSTITUTE OF TECHNOLOGY

3 Inria

4 université PARIS-SACLAY

5 vrvis

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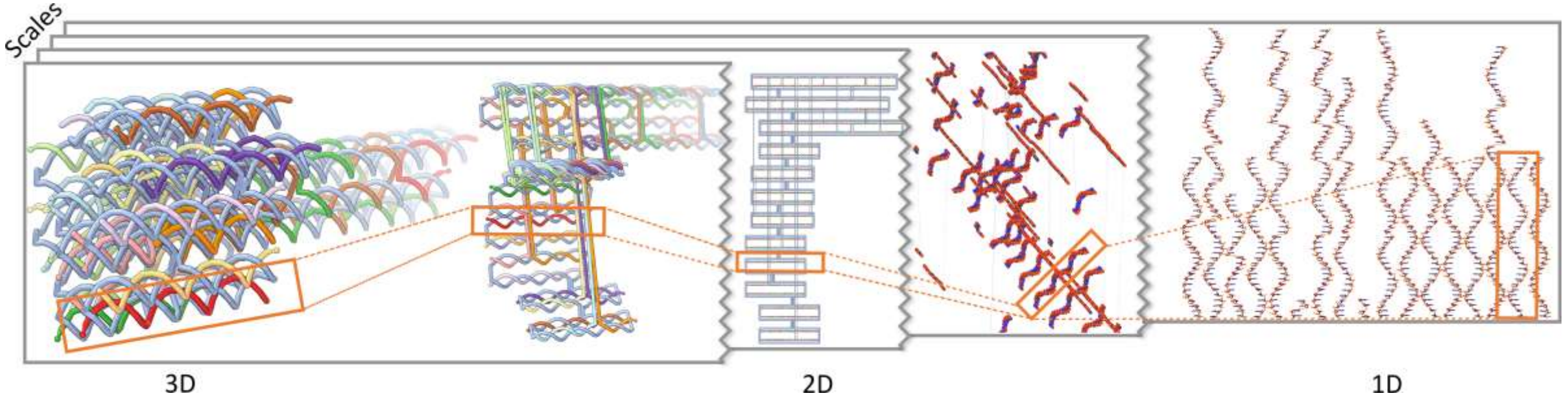


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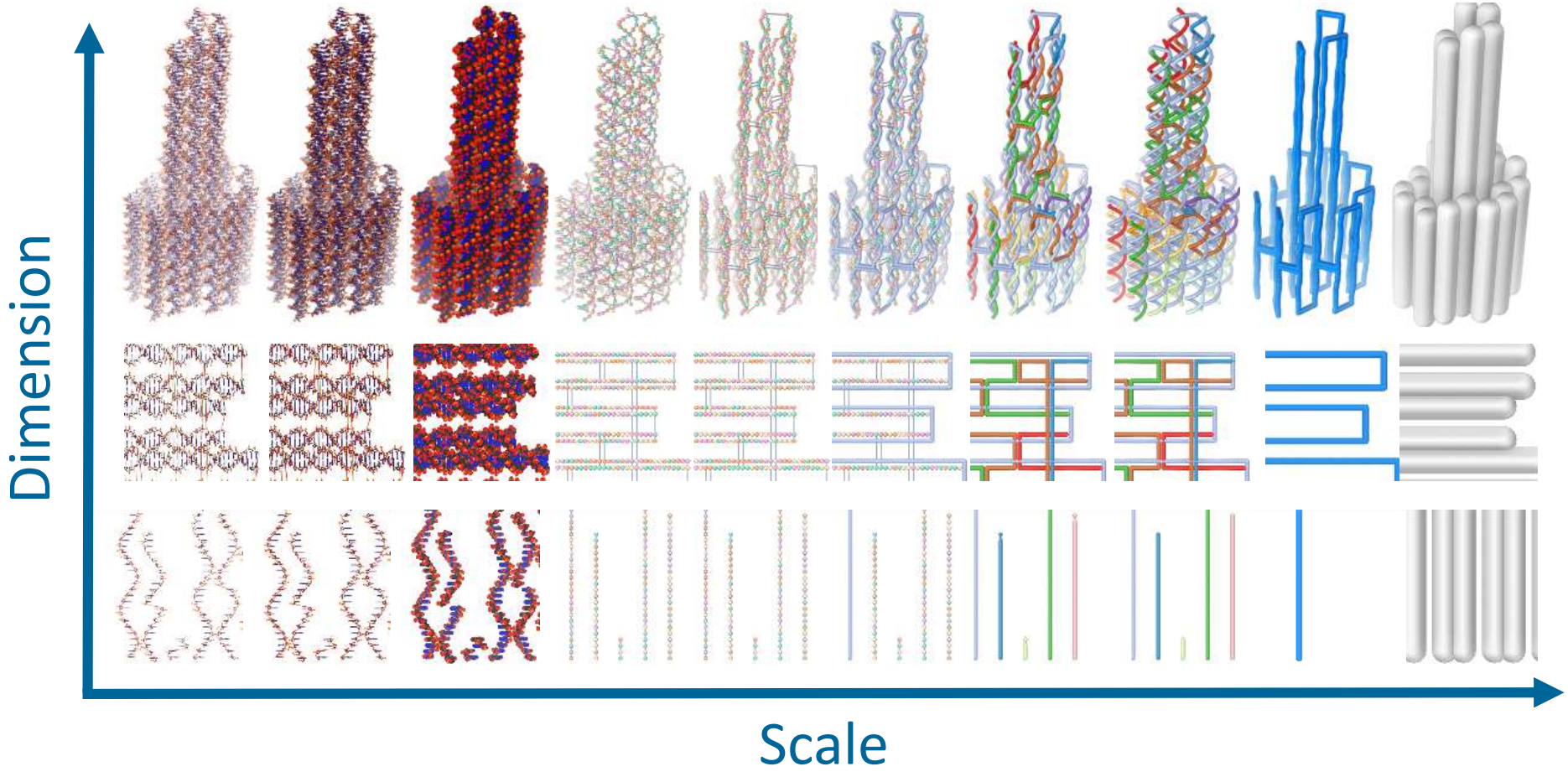
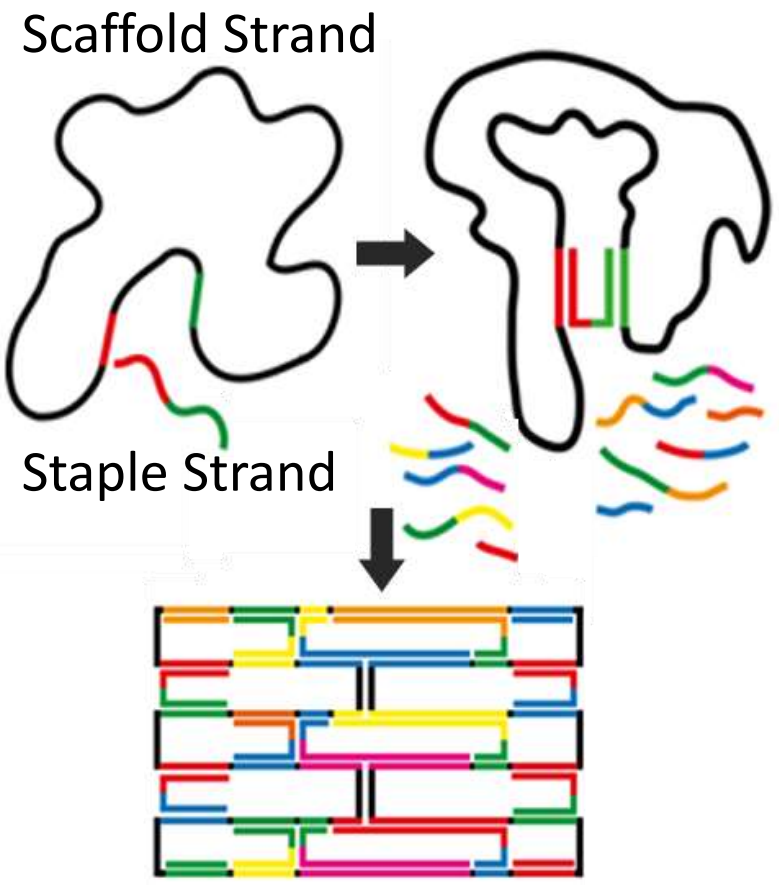


# DNA Origami Method




Modified from openwetware.org

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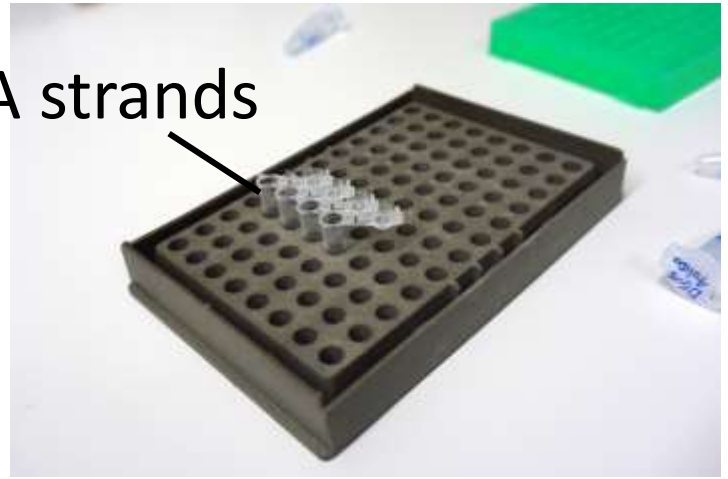
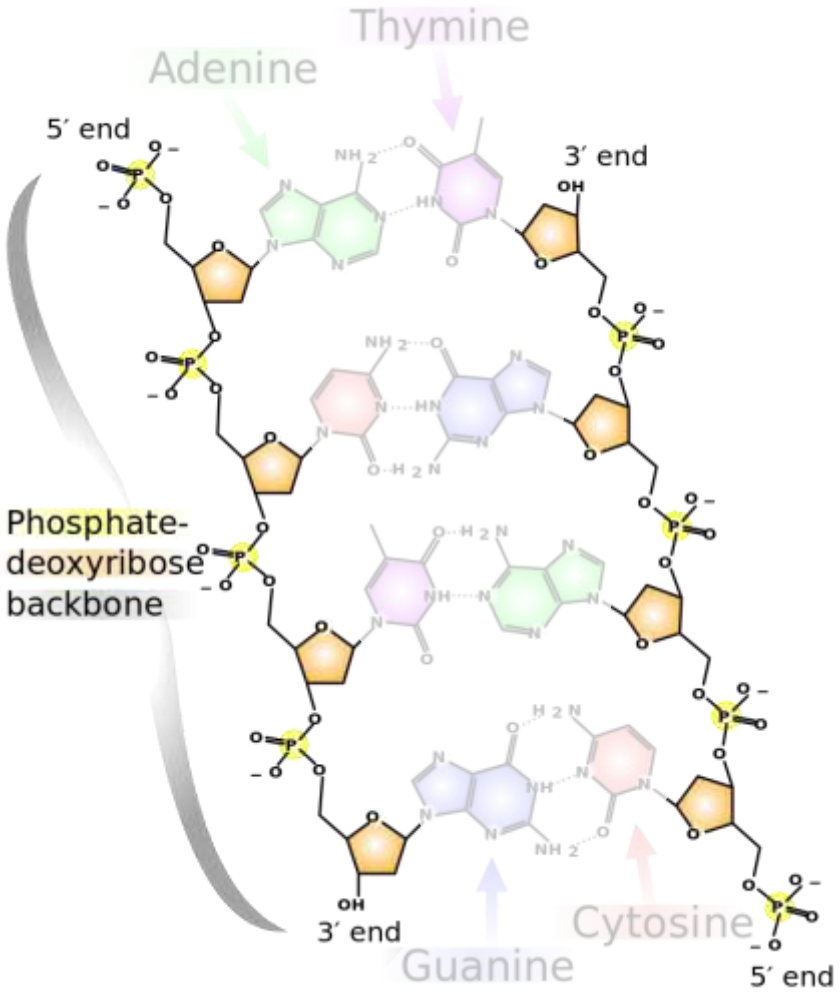
DNA strands



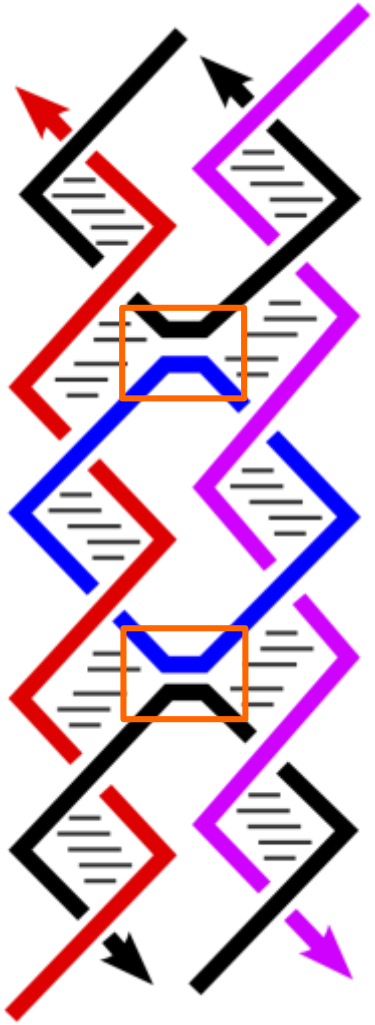

In Silico Design → DNA Sequence Export → Self-Assembly in the Lab

# DNA Origami | Conceptual Foundation



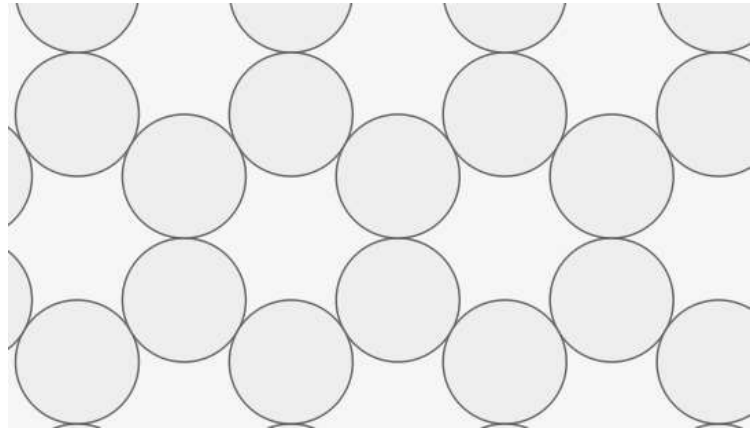

By Madeleine Price Ball

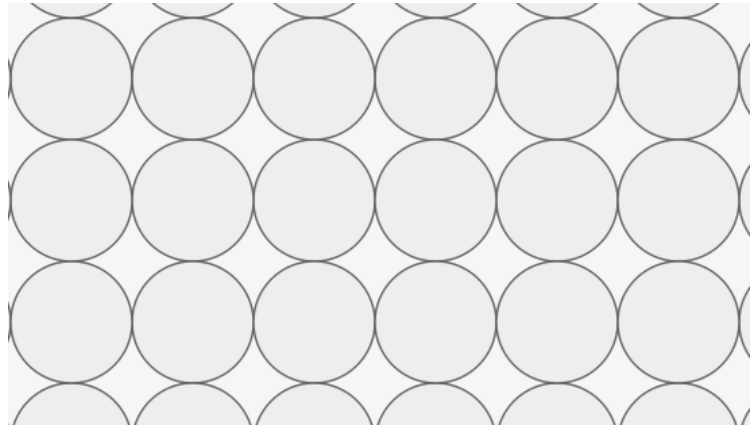
## Chemical Structure



Mao 2004

## Crossovers

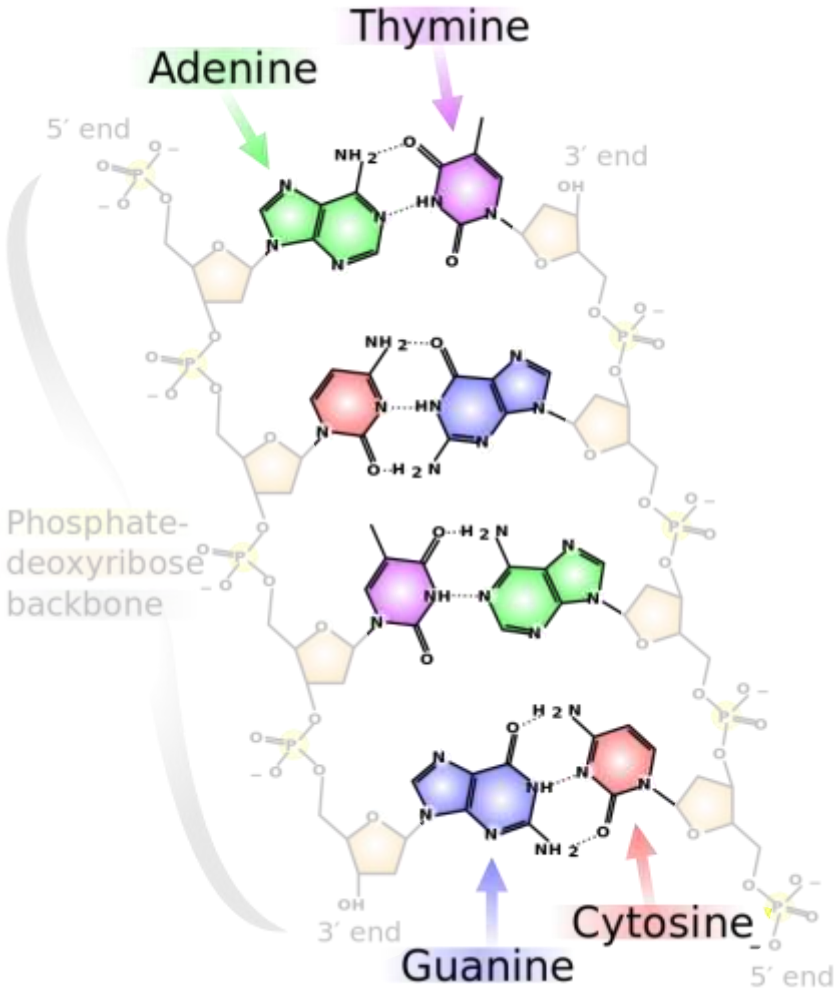




Douglas et al. 2009

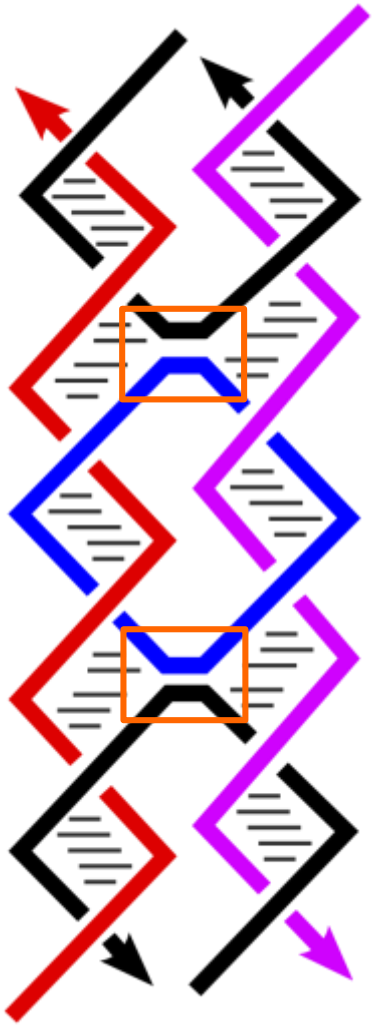
## Lattice Arrangement

# DNA Origami | Conceptual Foundation



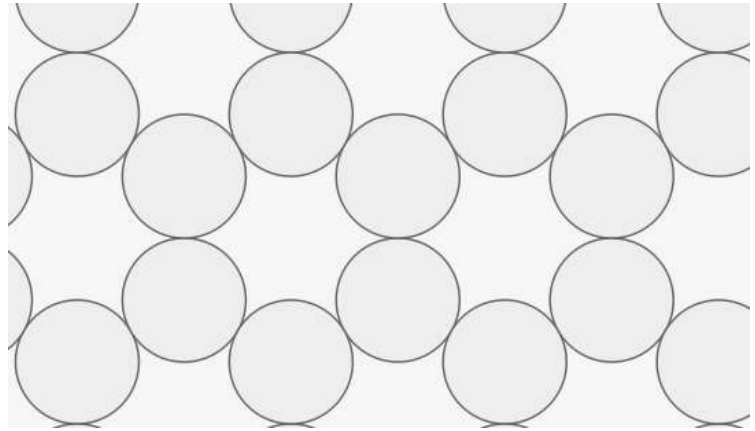

By Madeleine Price Ball

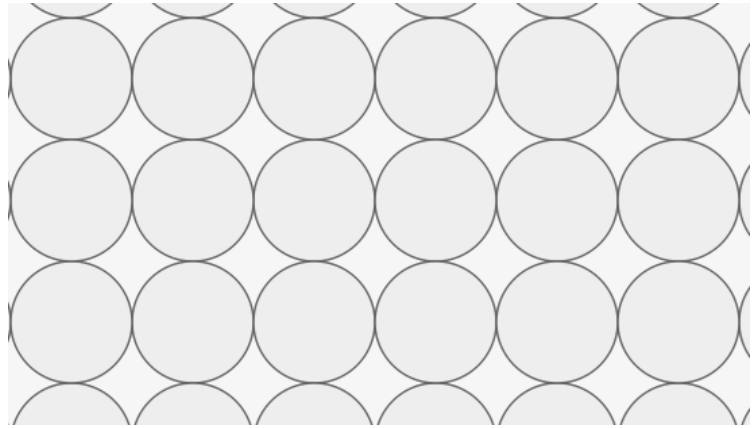
## Chemical Structure



Mao 2004

## Crossovers

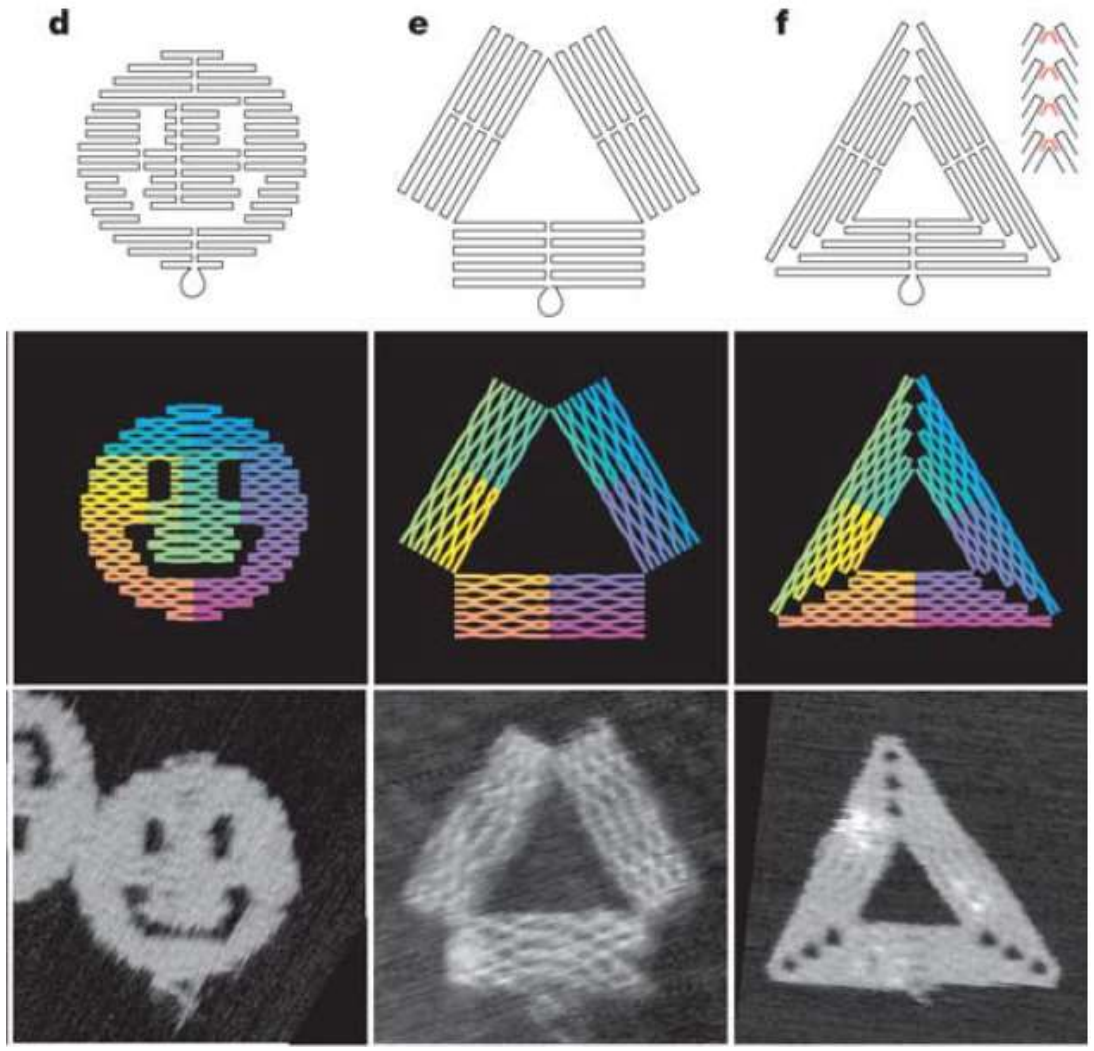




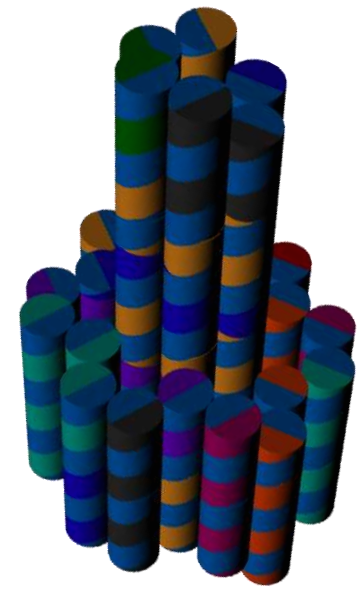
Douglas et al. 2009

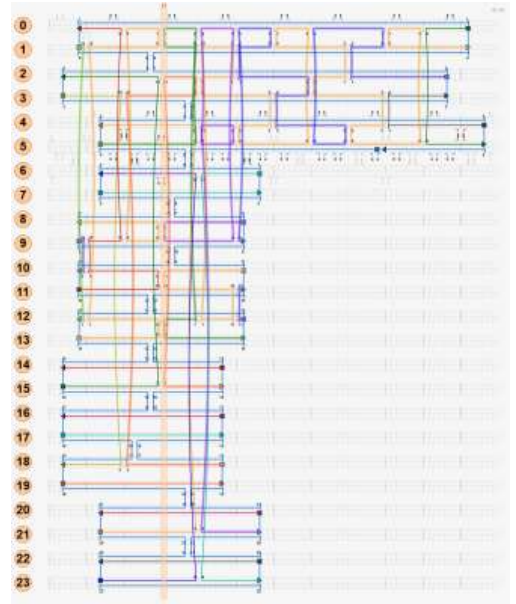
## Lattice Arrangement

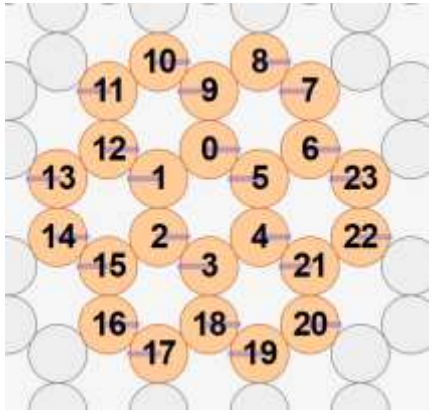
# State-of-the-art Method & Tool




Rothemund 2006








| Start | End | Sequence | Length |
|---|---|---|---|
| 15[2] | 2[2] | TCCGCTCACAATTCCACCATCCGATCGGTGCGGGCCTC | 38 |
| 1[5] | 12[5] | ACAT | 4 |
| 2[74] | 9[36] | ACAAACGGCGGATTGACCGGTATCGGGGCACCGCTTCTGGAAACC | 98 |
| 10[36] | 1[78] | AATCAAAAGAATAGTCGGCAAAATCCCTTAGATGGTGCATCTGCTC | 172 |
| 11[5] | 0[5] | CGGGTACCGAGCTCTCGACTCTAGAGGATCCTTGCATGGCTGCGC | 46 |
| 16[32] | 16[2] | CCCTGAGAGAGTTGACAACATACGAGCCGGA | 31 |
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| 14[32] | 14[2] | CGCTGGTTTGCCCCCCTGTGTGAAATTGTTA | 31 |
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| 22[39] | 22[9] | AGGCGGTTTGCGTAAAACCTGTCGTGCCAGC | 31 |
| 13[5] | 8[5] | GGTCATAGCTGTTTAGAAGAATTCGTAATCTGTTGGGAAGGGGTCC | 74 |
| 8[36] | 21[39] | GAGTGTTGTTCCAGAAGGCCCGAGATAGGGCAAAGCGACTCCAAC | 63 |
| 17[2] | 17[32] | AGCATAAAGTGTAATGCCCTTCACCGCCTGG | 31 |
| 18[32] | 15[32] | GACGGGCAACAGCTGATAGCCAGCTGGCGAAATGGGCGCAGCAA | 52 |
| 23[9] | 6[9] | TGCATTAATGAATCGGCCAGTACGCCAGGGTTTTCCCA | 38 |
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| 5[9] | 13[36] | GGCGATTAAGTTGGGTAGGCCATTCGAACCGTGGTTCCGACAGGC | 56 |
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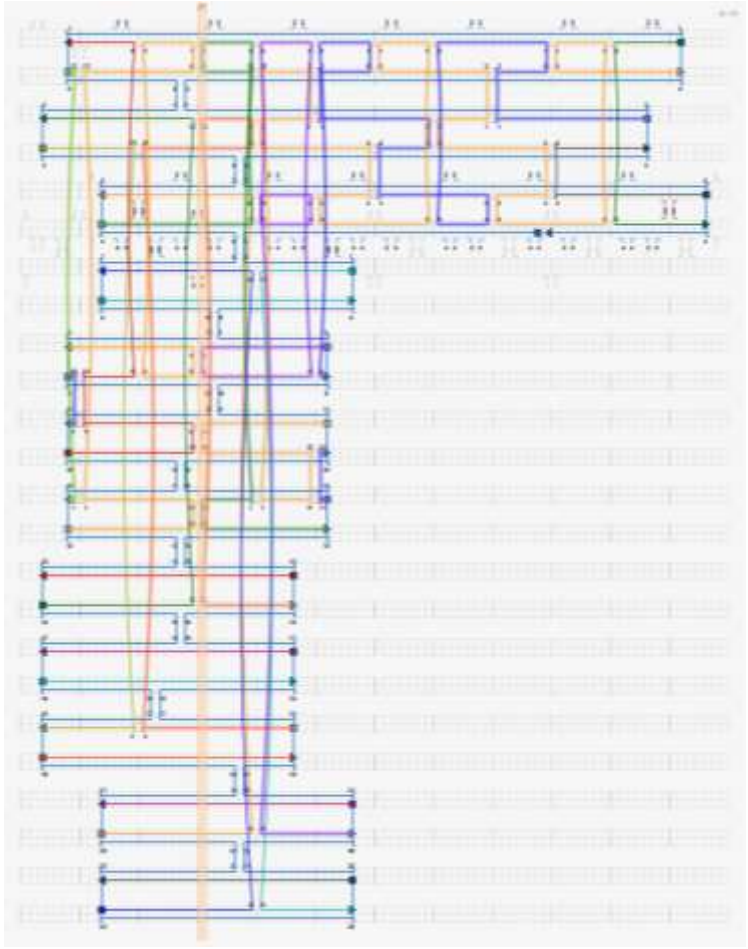
| 20[39] | 20[9] | GGTTTTTCTTTTCATTGCGTTGCGCTCACTG | 31 |
| 6[39] | 23[39] | CTATTAAAGAACACGCGCGGGGAG | 24 |
| 7[9] | 7[39] | GTCACGACGTTGTATTTGGAACAAGAGTCCA | 31 |

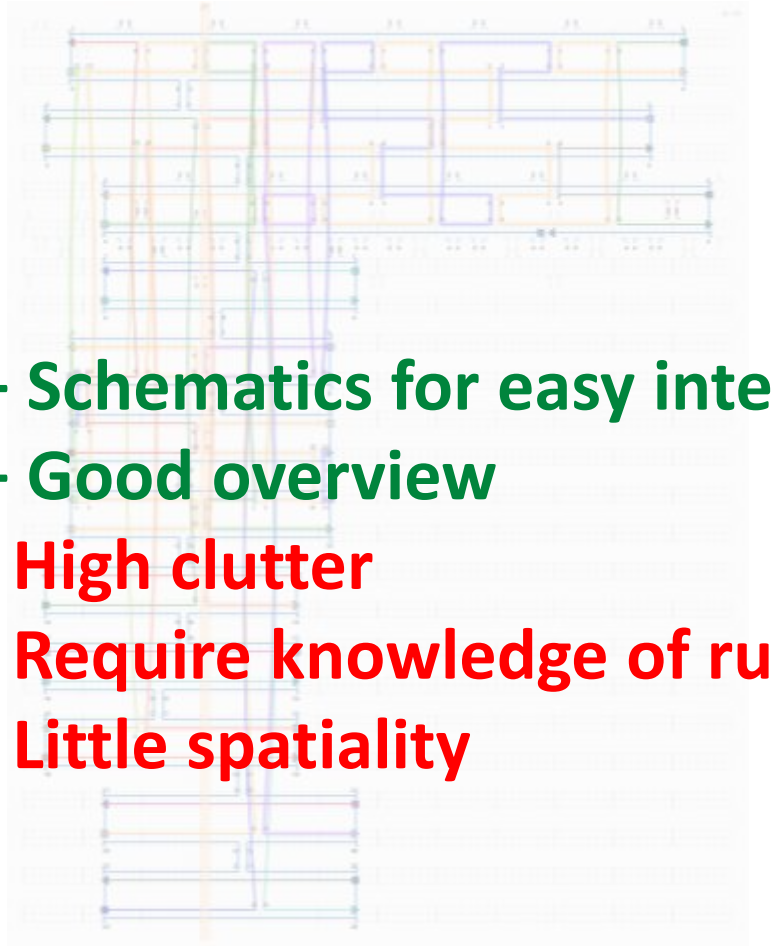
caDNAno by Douglas et al. 2009

# 2D | Schematics and Modeling



Douglas et al. 2009

# 2D | Schematics and Modeling



+ Schematics for easy interaction
+ Good overview
- High clutter
- Require knowledge of rules
- Little spatiality

Douglas et al. 2009

# 2D | Schematics and Modeling

+ Schematics for easy interaction
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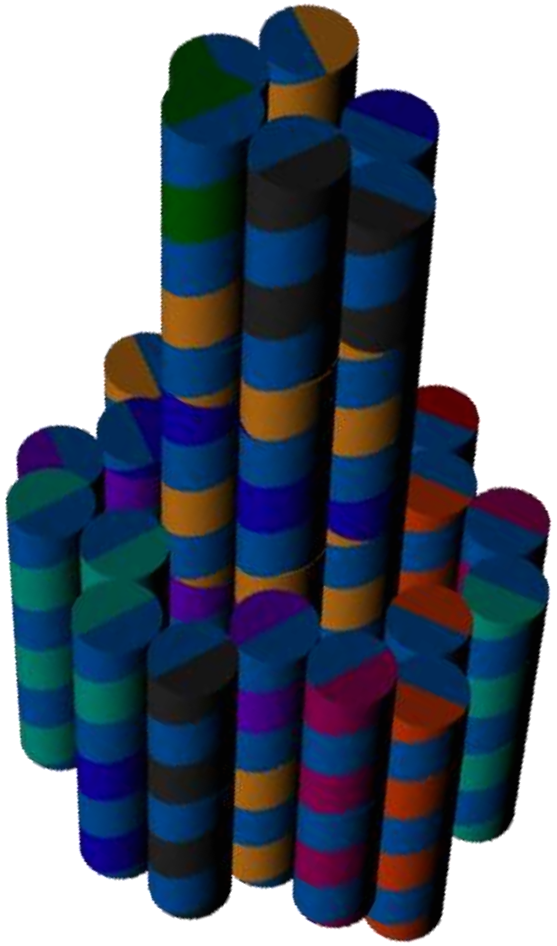
Douglas et al. 2009

# 3D | Spatial Features & Distances



Douglas et al. 2009

# 3D | Spatial Features & Distances

+ Realistic spatial arrangement

- Visual occlusion

- Hard to examine individual strands

Douglas et al. 2009

# 1D | Sequences

| Start | End | Sequence | Length |
|---|---|---|---|
| 15[2] | 2[2] | TCCGCTCACAATTCCACCATCCGATCGGTGCGGGCCTC | 38 |
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| 21[9] | 4[9] | CCCGCTTTCCAGTCGGGTTTCAGGGGGATGTGCTGCAA | 38 |
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| 13[5] | 8[5] | GGTCATAGCTGTTTAGAAGAATTCGTAATCTGTTGGGAAGGGGTCC | 74 |
| 8[36] | 21[39] | GAGTGTTGTTCCAGAAGGCCCGAGATAGGGCAAAGCGACTCCAAC | 63 |
| 17[2] | 17[32] | AGCATAAAGTGTAATGCCCTTCACCGCCTGG | 31 |
| 18[32] | 15[32] | GACGGGCAACAGCTGATAGCCAGCTGGCGAAATGGGCGCAGCAAC | 52 |
| 23[9] | 6[9] | TGCATTAATGAATCGGCCAGTACGCCAGGGTTTTCCCA | 38 |
| 0[78] | 5[81] | CTCCAGCCACTCATTTTTTAA | 21 |
| 5[9] | 13[36] | GGCGATTAAGTTGGGTAGGCCATTCGAACCGTGGTTCCGACAGGC | 56 |
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| 20[39] | 20[9] | GGTTTTTCTTTTCATTGCGTTGCGCTCACTG | 31 |
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| 11[5] | 10[5] | AC | 4 |
| 12[36] | 11[36] | TTTA | 4 |
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| 22[9] | 22[9] | AACCTGTCGTGCCAGC | 31 |
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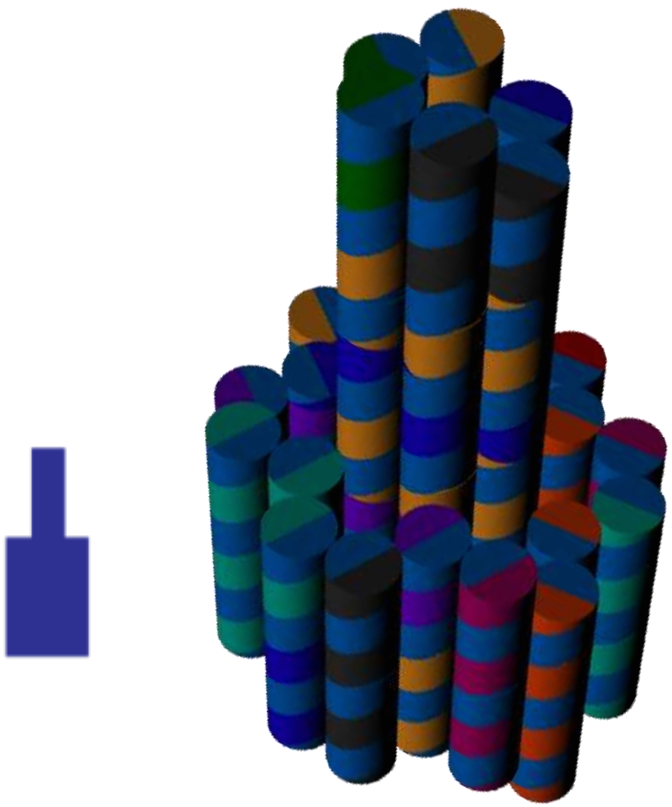
| 6[39] | 23[39] | CTATTAAAGAACACGCGCGGGGAG | 24 |
| 7[9] | 7[39] | GTCACGACGTTGTATTTGGAACAAGAGTCCA | 31 |

**+ Clean arrangement of strands**

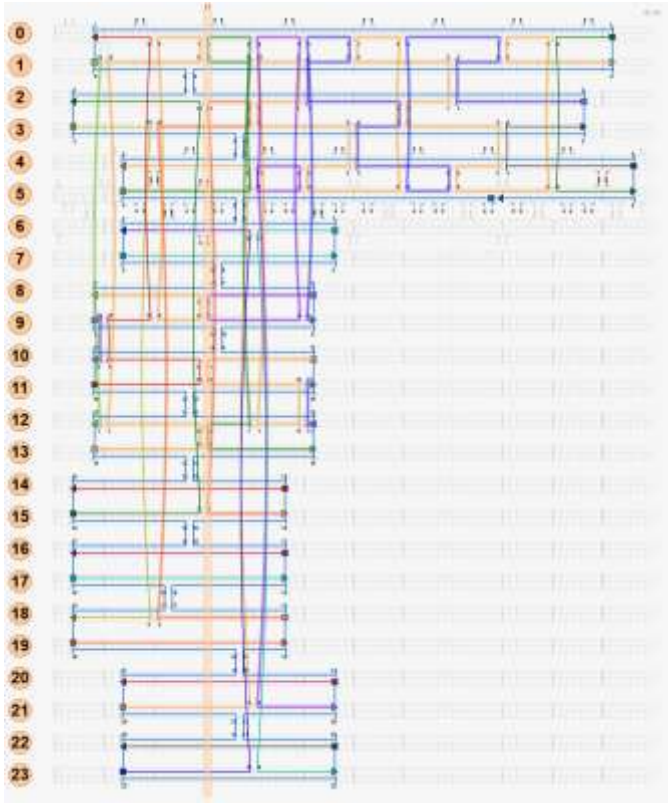
**+ Sorting of strands**

**- No spatiality**

# Modeling and Inspection



3D



2D

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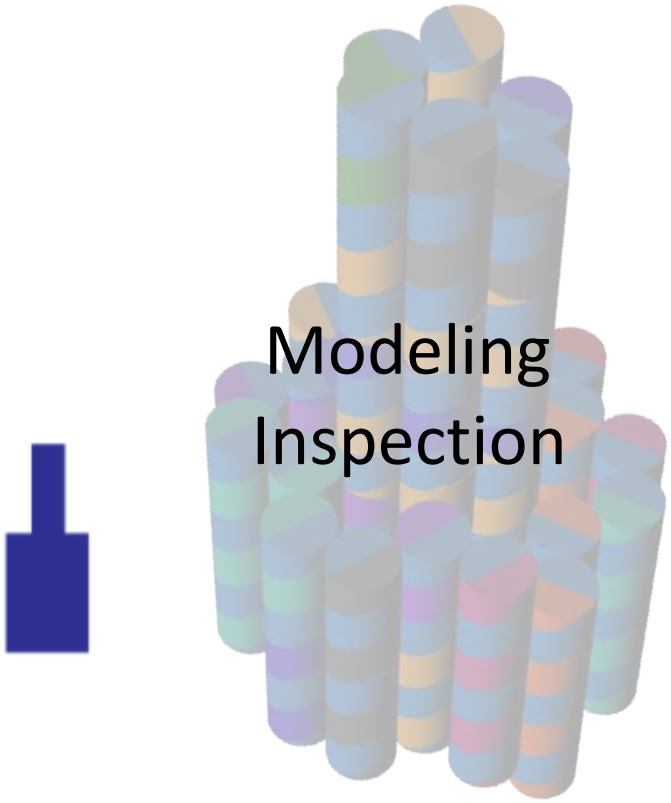
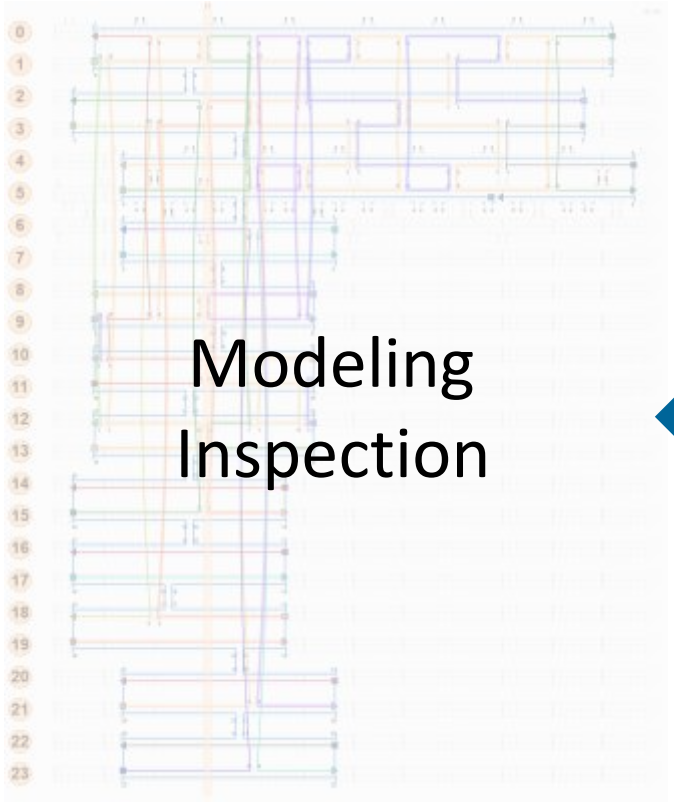
1D

# Modeling and Inspection

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| 19[2] | 19[32] | AATGAGTC | 31 |
| 14[32] | 14[2] | CGCTGGTT | 31 |
| 21[9] | 4[9] | CCCGCTTTCCAGTCGGGTTTCAGGGGGATGTGCTGCAA | 38 |
| 22[39] | 22[9] | AGGCGG | 31 |
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| 17[2] | 17[32] | AGCATAAAGTGTAATGCCCTTCACCGCCTGG | 31 |
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| 7[9] | 7[39] | GTCACGACGTTGTATTTGGAACAAGAGTCCA | 31 |

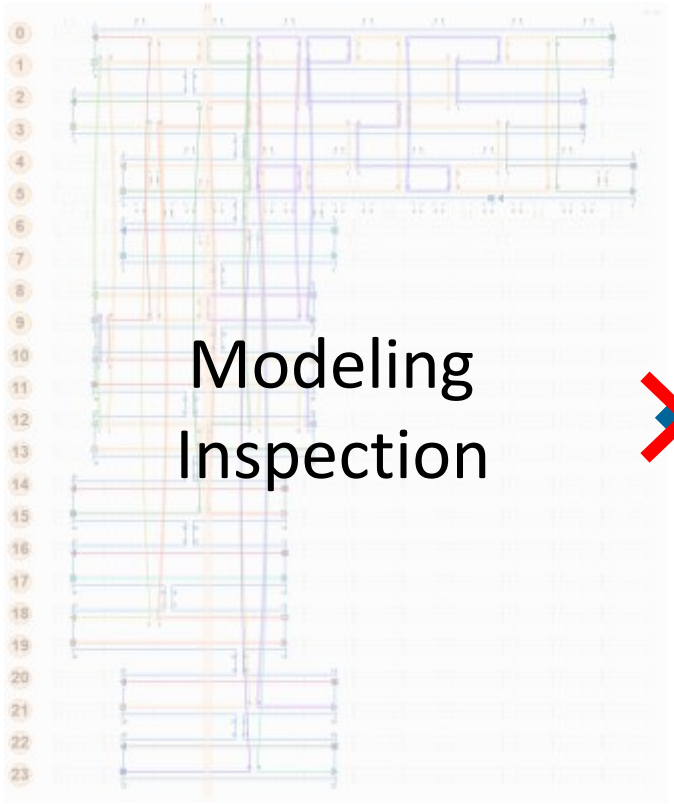
Modeling
Inspection

3D 2D 1D

# Modeling and Inspection

~~Modeling~~
Inspection

3D



Modeling
Inspection

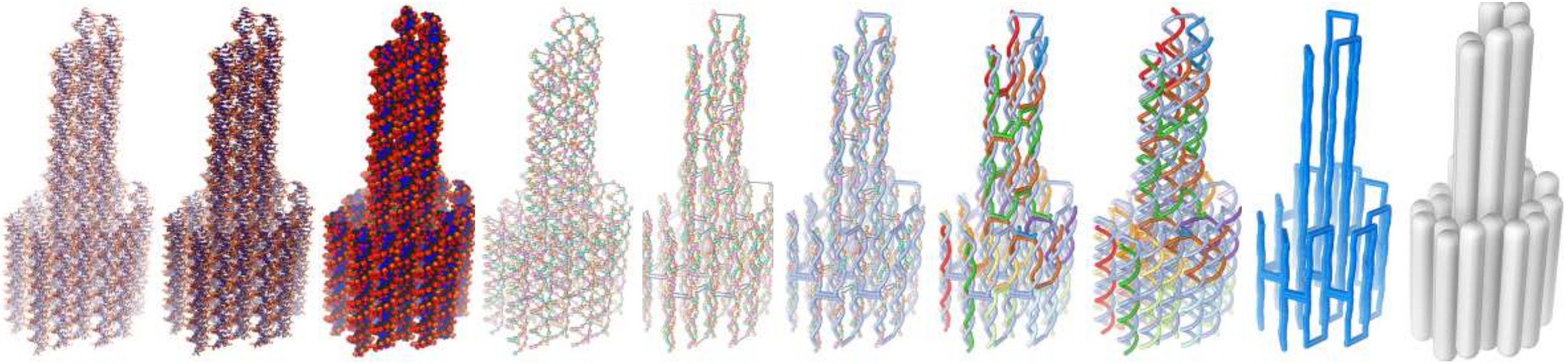
2D

| Start | End | Sequence | Length |
|---|---|---|---|
| 15[2] | 2[2] | TCCGCTCACAATTCCACCATCCGATCGGTGCGGGCCTC | 38 |
| 1[5] | 12[5] | ACAT | 4 |
| 2[74] | 9[36] | ACAAACGGCGGATTGACCGGTATCGGGGCACCGCTTCTGGAAACC | 98 |
| 10[36] | 1[78] | AATCAAAAGAATAGTCGGCAAAATCCCTTAGATGGTGCATCTGCTC | 172 |
| 11[5] | 0[5] | CGGGTACCGAGCTCTCGACTCTAGAGGATCCTTGCATGGCTGCGC | 46 |
| 16[32] | 16[2] | CCCTGAGAGAGTTGACAACATACGAGCCGGA | 31 |
| 4[81] | 3[74] | CCAATAGGAACGCCATCAATTCTCCGTGGGA | 31 |
| 9[5] | 10[5] | AGCC | 4 |
| 12[36] | 11[36] | TTTA | 4 |
| 19[2] | 19[32] | AATGAGTC | 31 |
| 14[32] | 14[2] | CGCTGGTT | 31 |
| 21[9] | 4[9] | CCCGCTTTCCA GGGTTTCAGGGGGA TGCTGCAA | 38 |
| 22[39] | 22[9] | AGGCGG TTGCGTAAAACCTGTCGT CAGC | 31 |
| 13[5] | 8[5] | GGTCATA GGAAGGGGTC | 74 |
| 8[36] | 21[39] | GAGTGTTGTTCCAGAAGGCCCGAGATAGGGCAAAGCGACTCCAAC | 63 |
| 17[2] | 17[32] | AGCATAAAGTGTAATGCCCTTCACCGCCTGG | 31 |
| 18[32] | 15[32] | GACGGGCAACAGCTGATAGCCAGCTGGCGAAATGGGCGCAGCAA | 52 |
| 23[9] | 6[9] | TGCATTAATGAATCGGCCAGTACGCCAGGGTTTTCCCA | 38 |
| 0[78] | 5[81] | CTCCAGCCACTCATTTTTTAA | 21 |
| 5[9] | 13[36] | GGCGATTAAGTTGGGTAGGCCATTCGAACCGTGGTTCCGACAGGC | 56 |
| 3[2] | 18[2] | TTCGCTATTACGCCTGGGGTGCCT | 24 |
| 20[39] | 20[9] | GGTTTTTCTTTTCATTGCGTTGCGCTCACTG | 31 |
| 6[39] | 23[39] | CTATTAAAGAACACGCGCGGGGAG | 24 |
| 7[9] | 7[39] | GTCACGACGTTGTATTTGGAACAAGAGTCCA | 31 |

~~Modeling~~
Inspection

1D

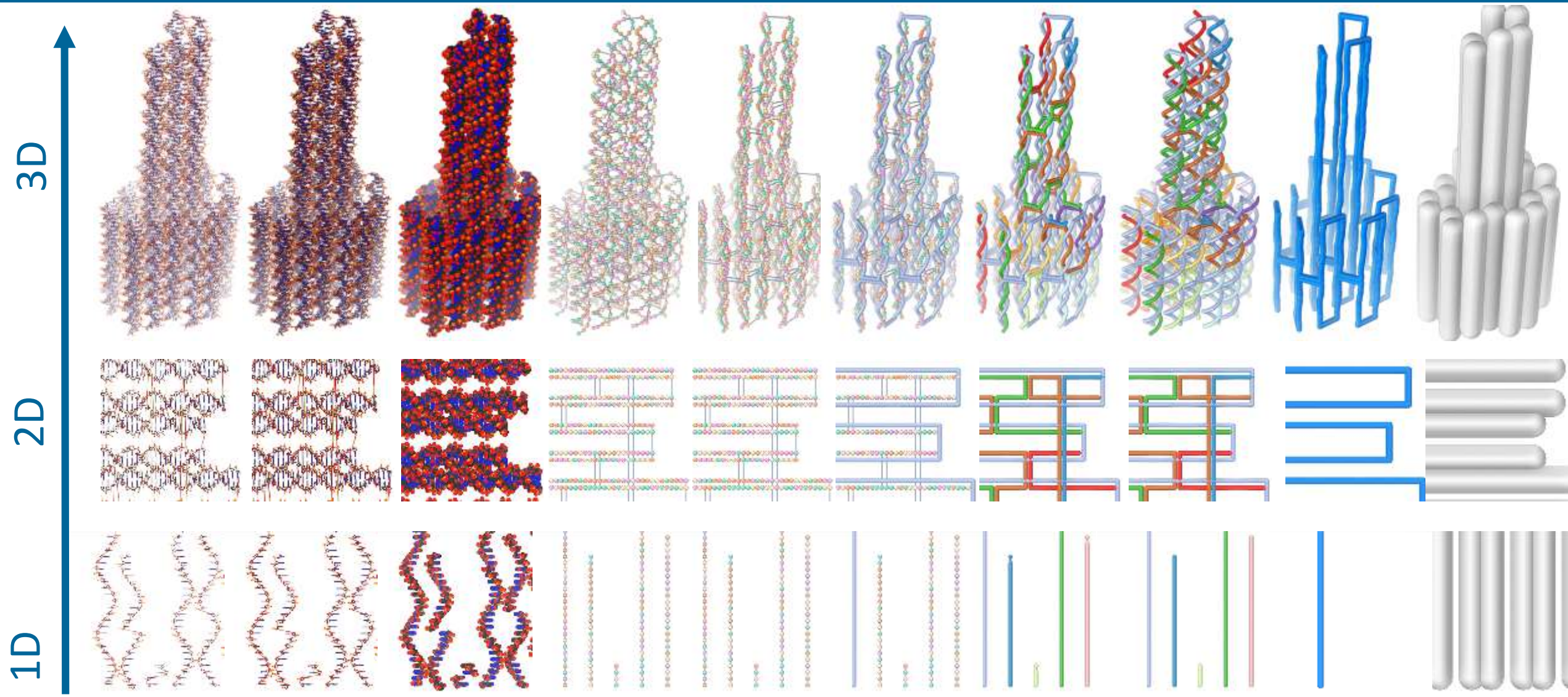
# Scale



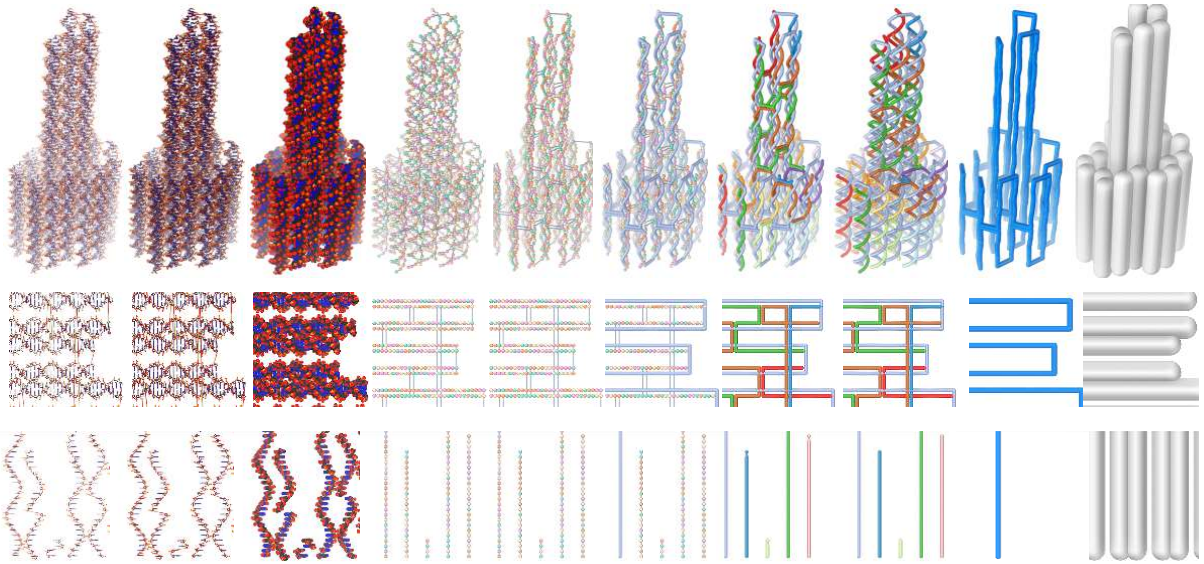
10 Scales

Miao et al. 2018

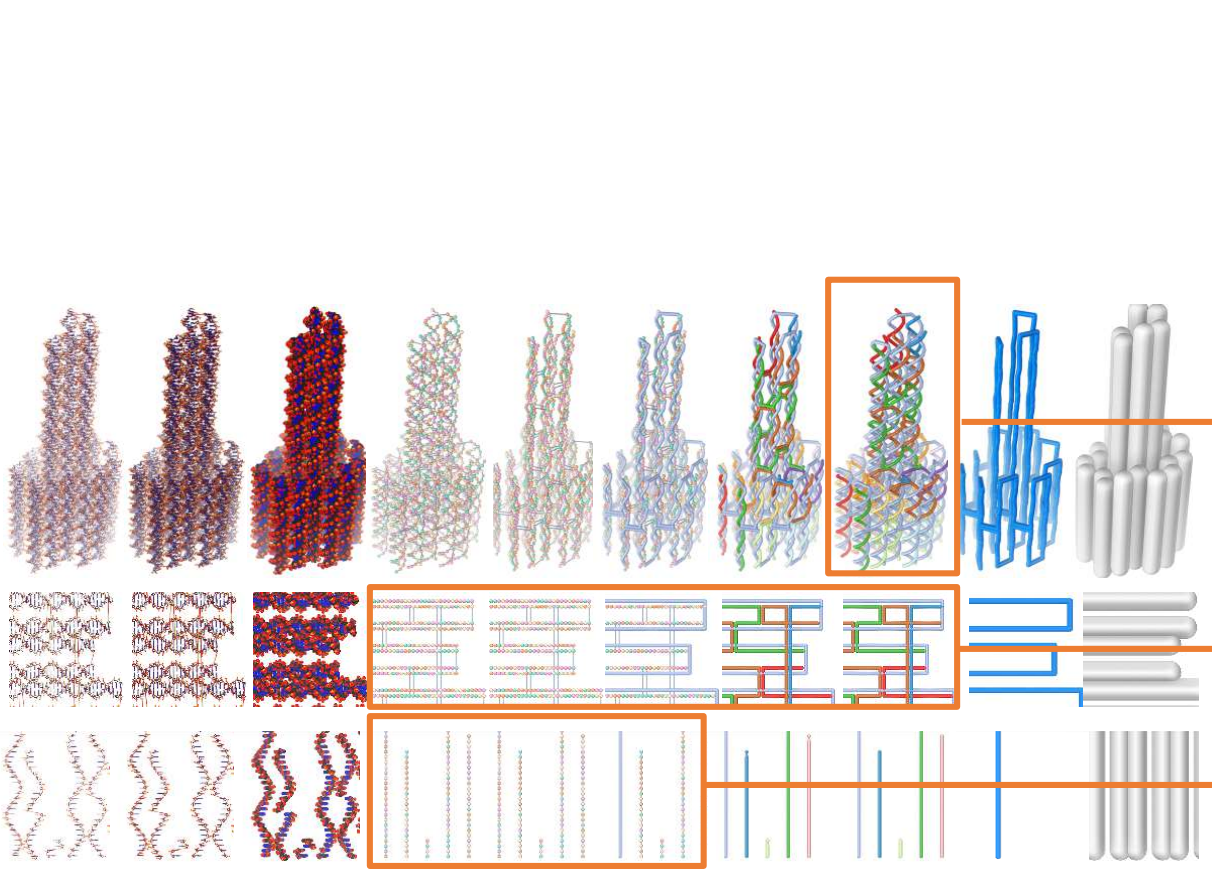
# Dimension and Scale

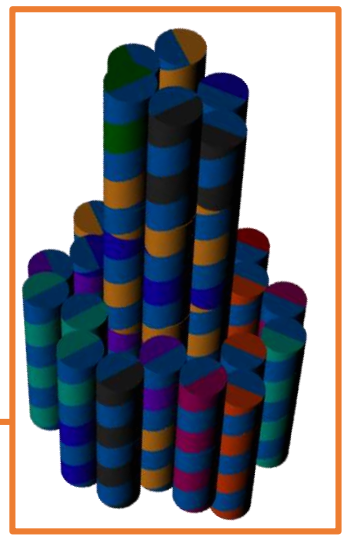


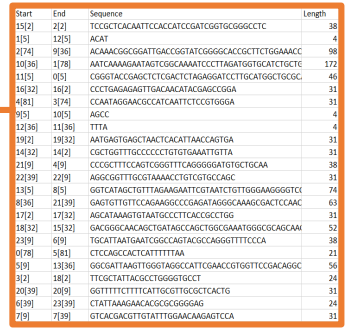
# Dimension and Scale Unifying Map (DimSUM)



# Dimension and Scale Unifying Map (DimSUM)







| Start | End | Sequence | Length |
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| 11[5] | 0[5] | CGGGTACCGAGCTCTCGACTCTAGAGGATCCTTGCATGGCTGCGC | 46 |
| 16[32] | 16[2] | CCCTGAGAGAGTTGACAACATACGAGCCGGA | 31 |
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| 8[36] | 21[39] | GAGTGTTGTTCCAGAAGGCCCGAGATAGGGCAAAGCGACTCCAAC | 63 |
| 17[2] | 17[32] | AGCATAAAGTGTAATGCCCTTCACCGCCTGG | 31 |
| 18[32] | 15[32] | GACGGGCAACAGCTGATAGCCAGCTGGCGAAATGGGCGCAGCAA | 52 |
| 23[9] | 6[9] | TGCATTAATGAATCGGCCAGTACGCCAGGGTTTTCCCA | 38 |
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| 5[9] | 13[36] | GGCGATTAAGTTGGGTAGGCCATTCGAACCGTGGTTCCGACAGGC | 56 |
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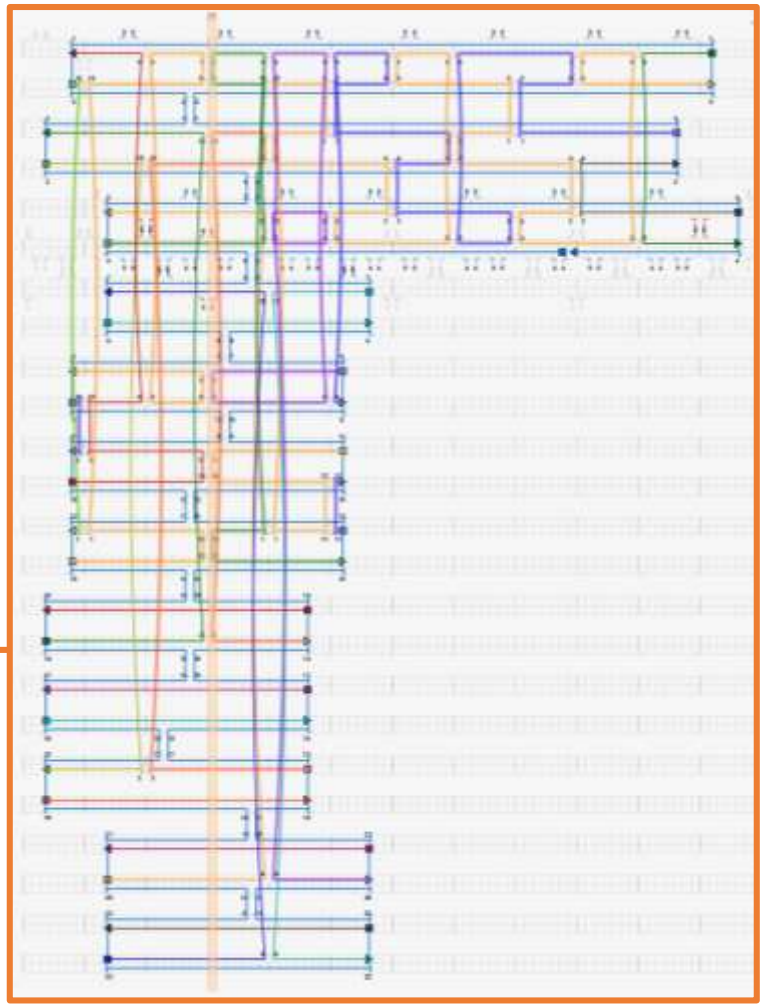
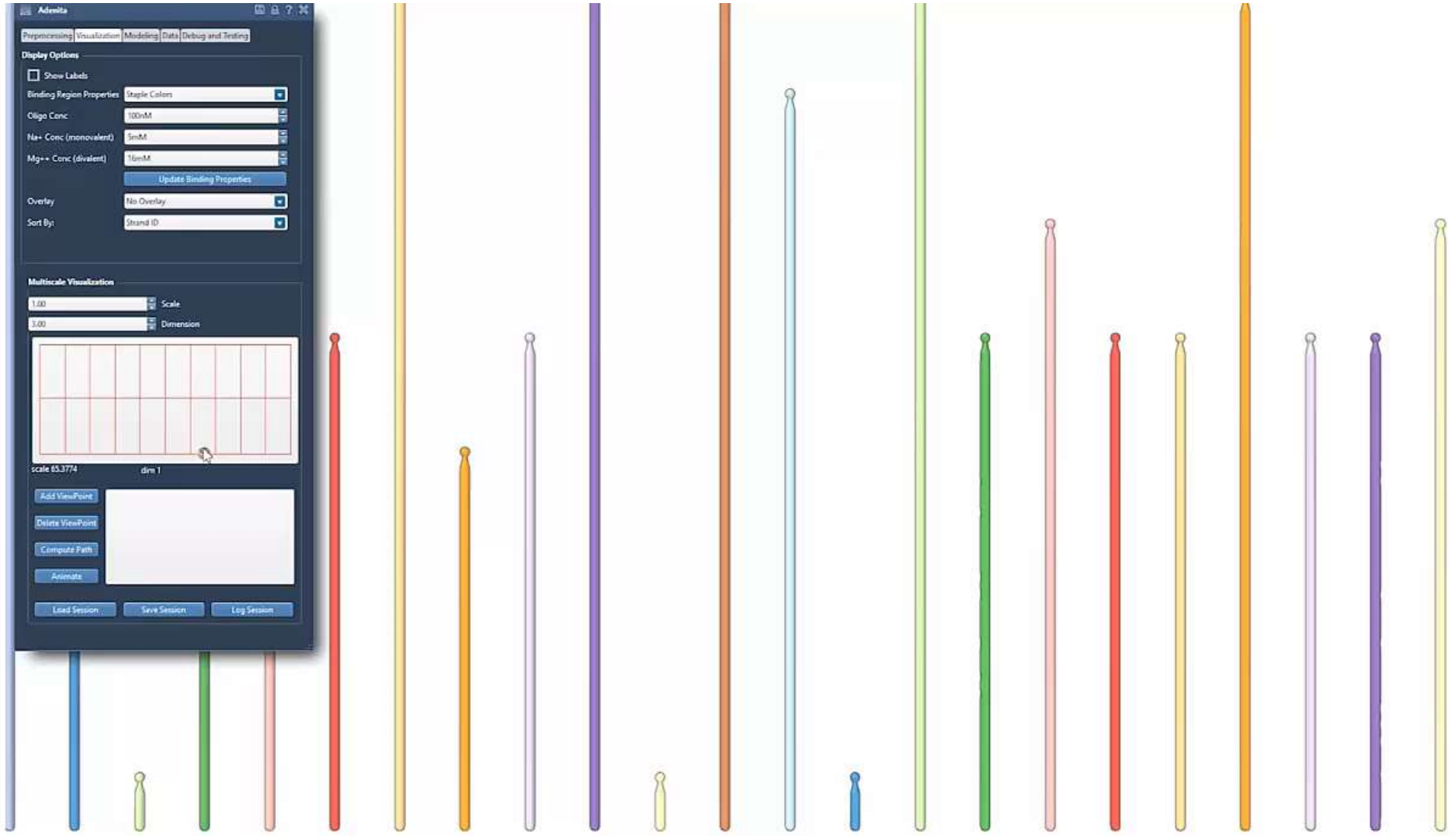
| 7[9] | 7[39] | GTCACGACGTTGTATTTGGAACAAGAGTCCA | 31 |

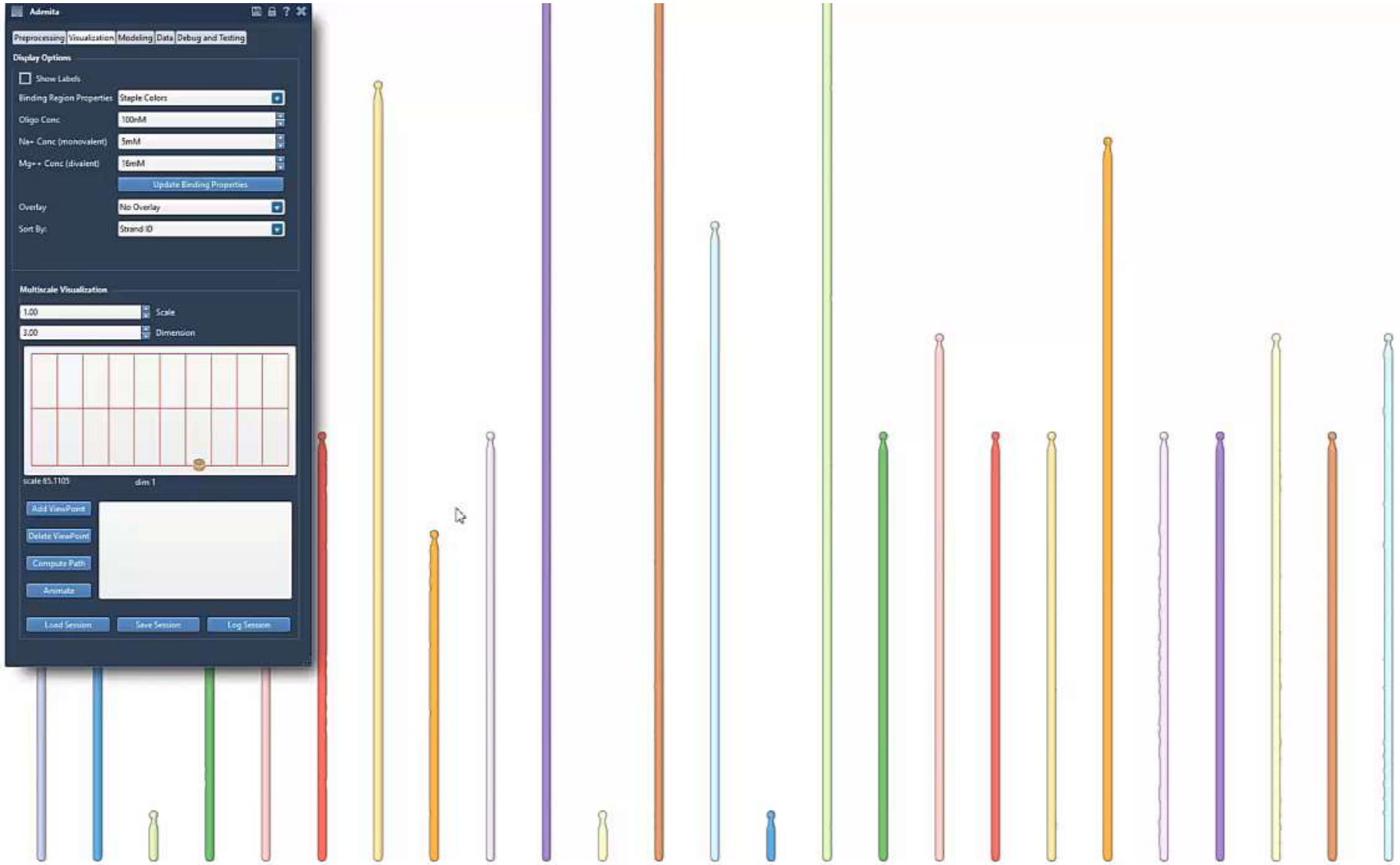


State-of-the-art by Douglas et al. 2009

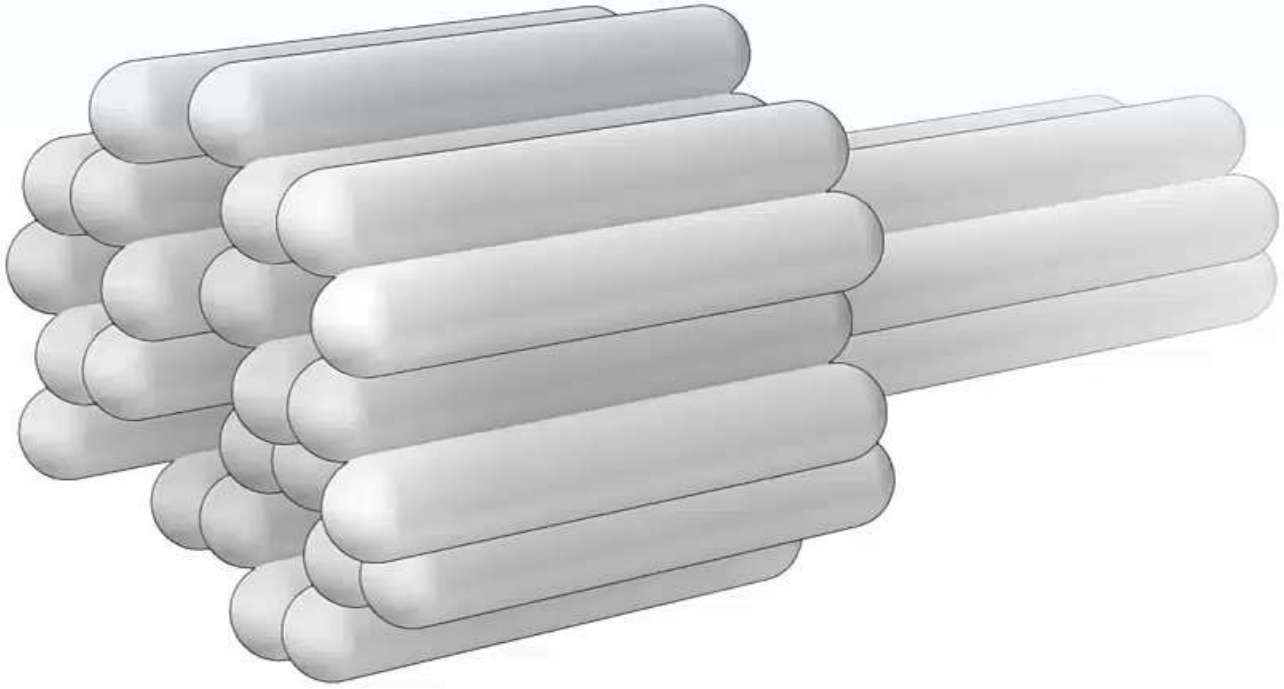
# Dimension and Scale Unifying Map (DimSUM)



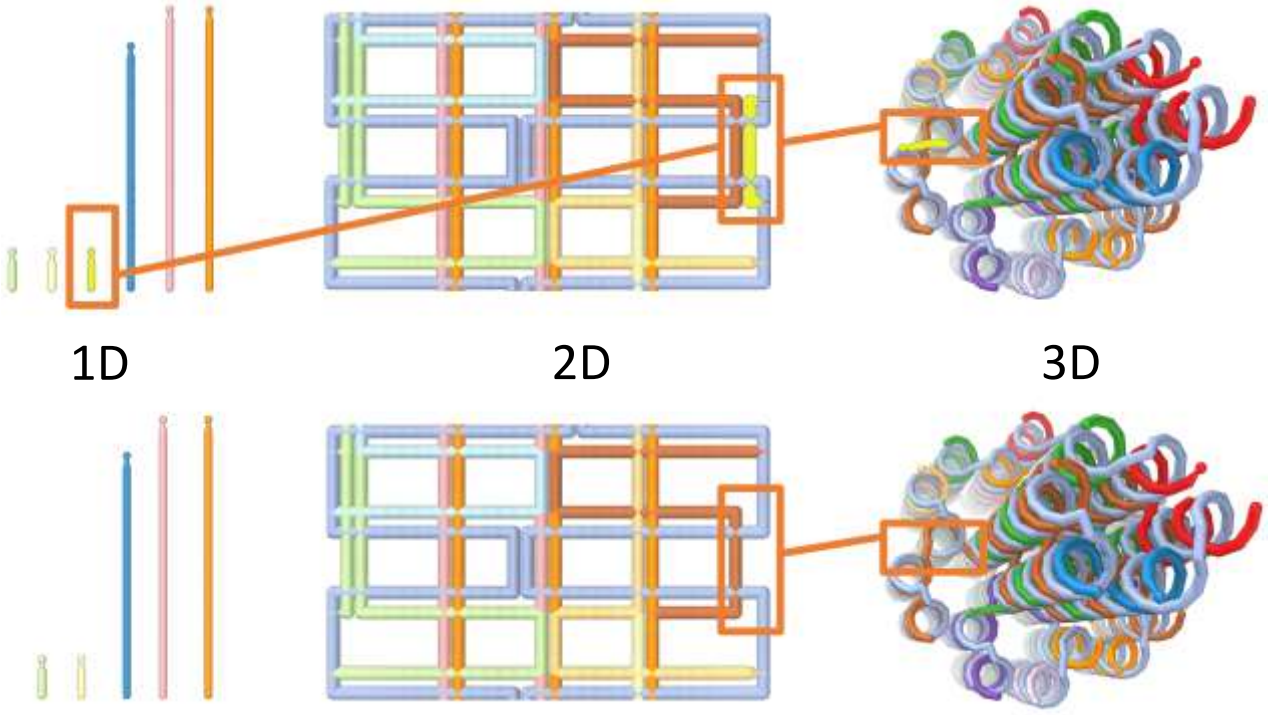
# Cross Dimension and Scale Highlighting



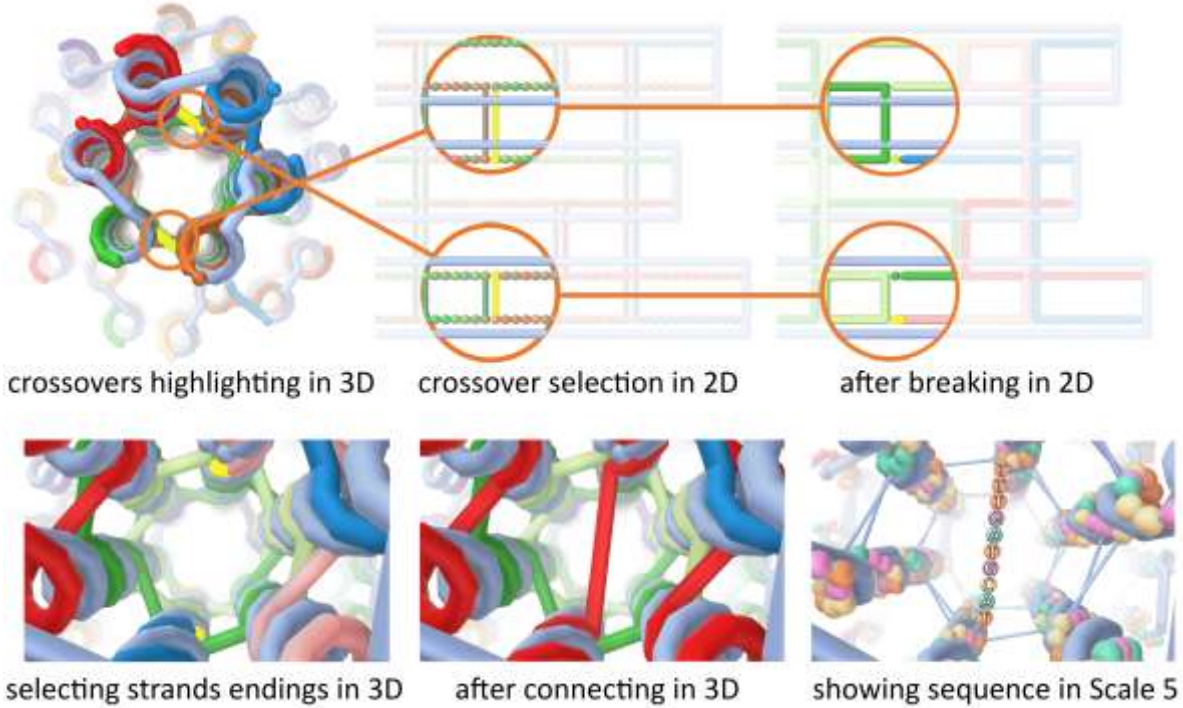
# Automated Feature Highlighting and Sorting

# Abstraction-adaptive Modifications

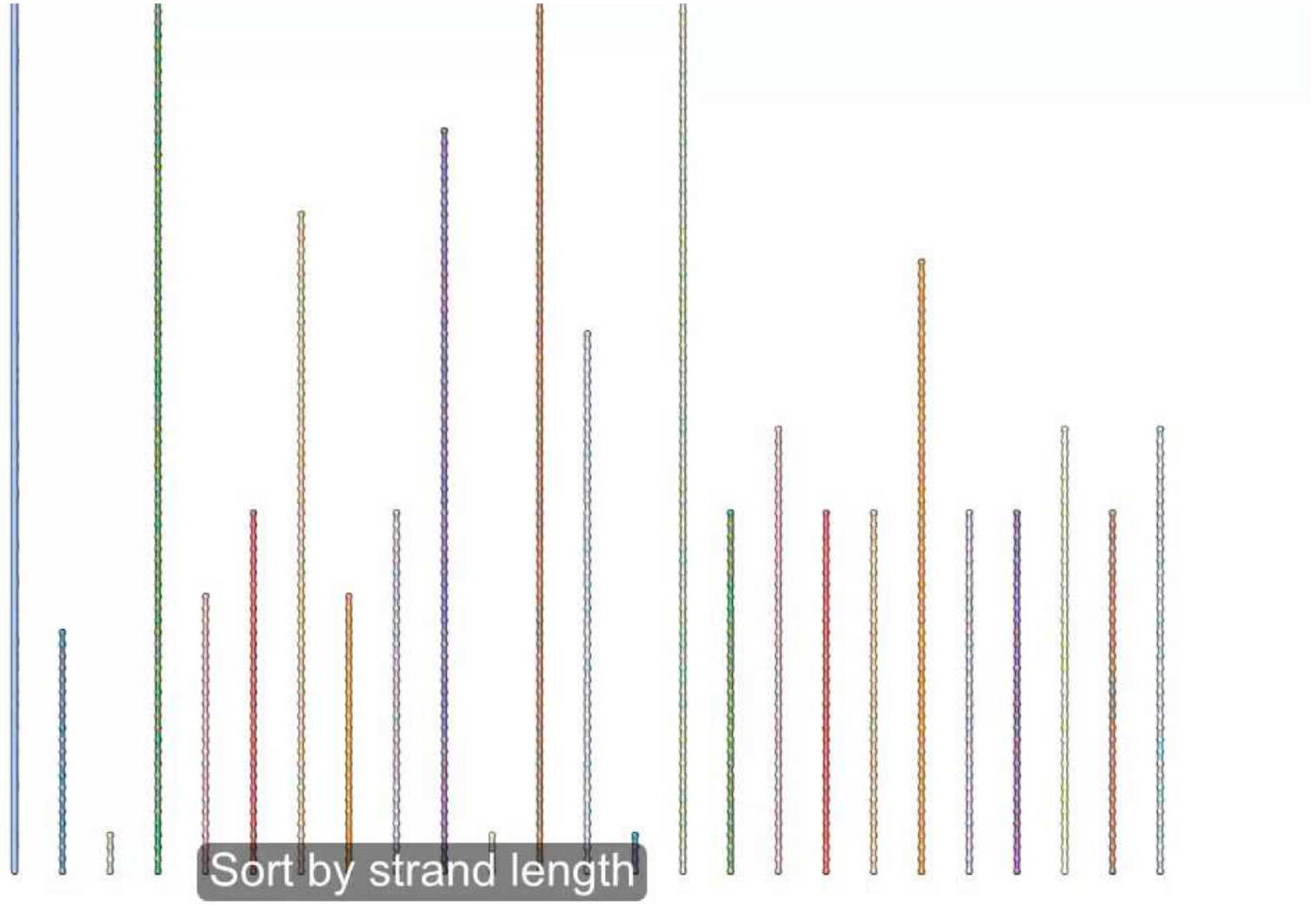



Task 1: Removing Short Staple Strands

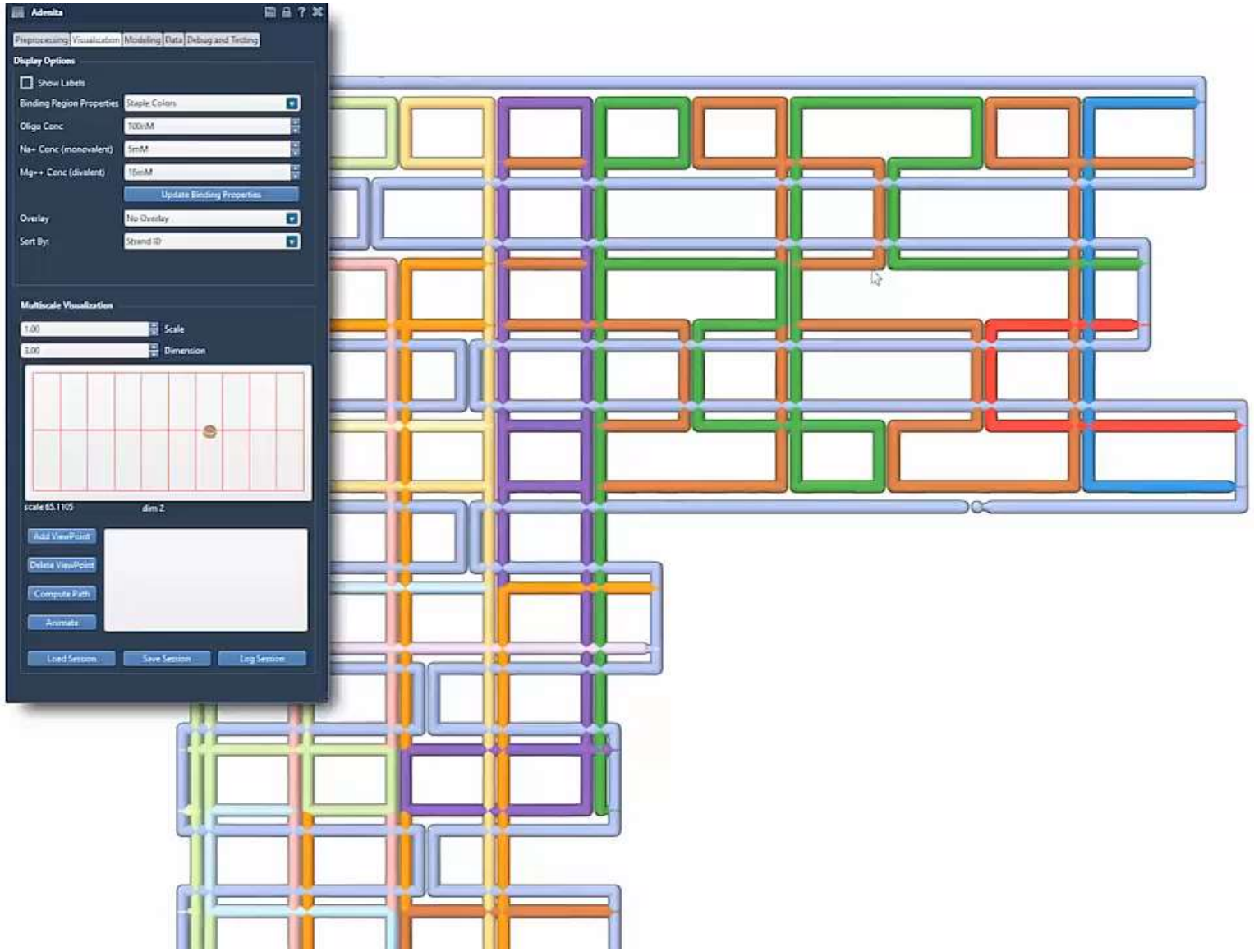



Task 2: Adding Bridging Strands

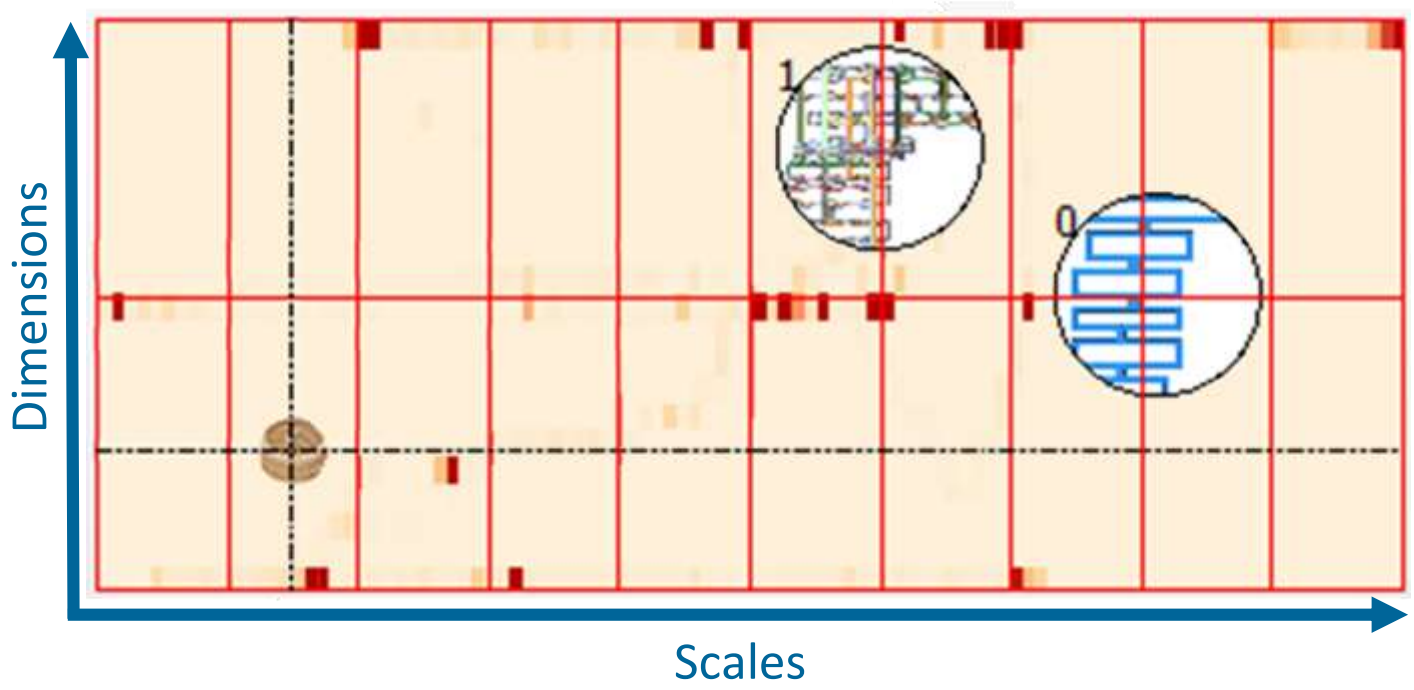
# Task 1: Removing Short Staple Strands

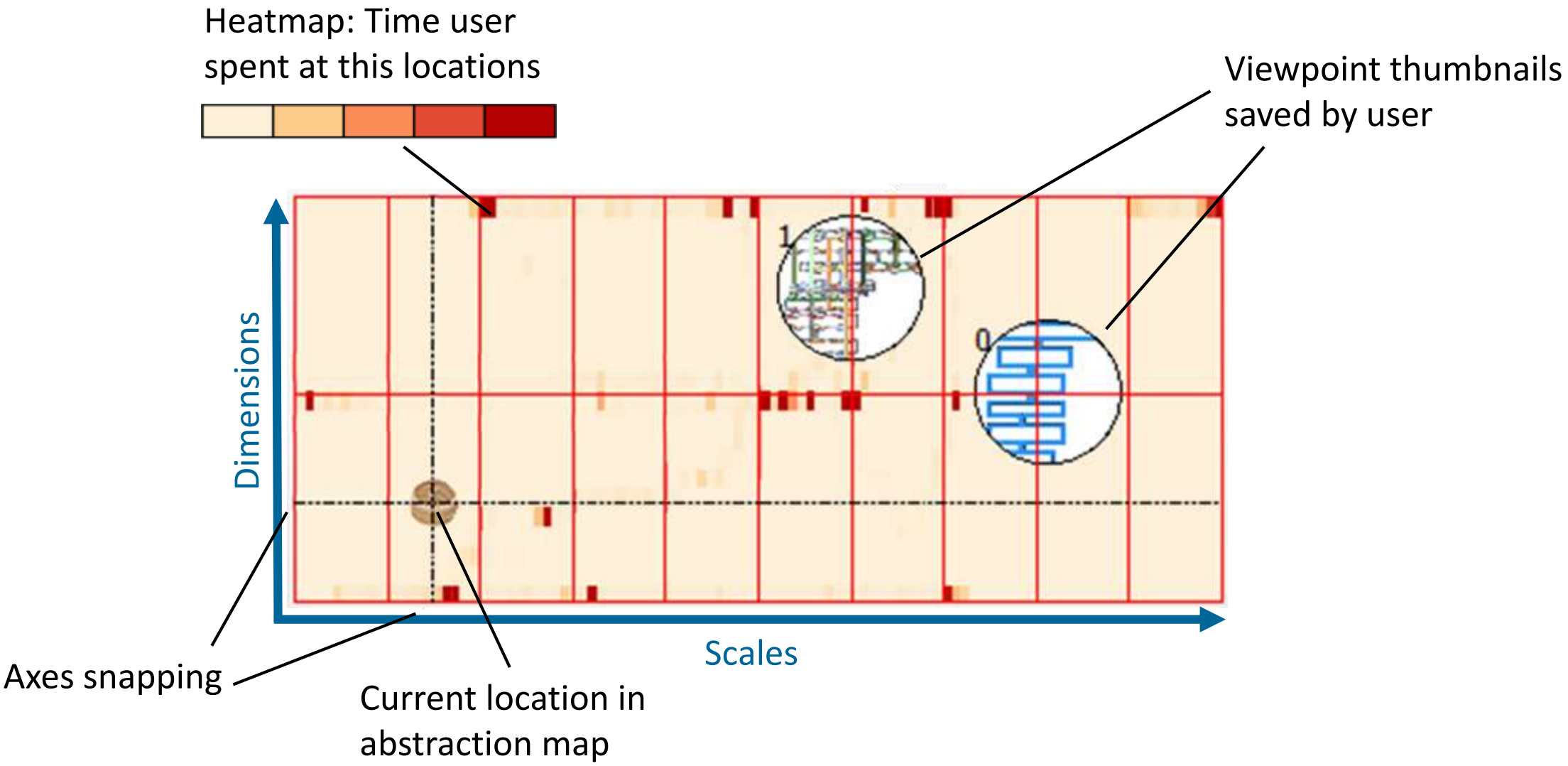
# Task 2: Adding Bridging Strands



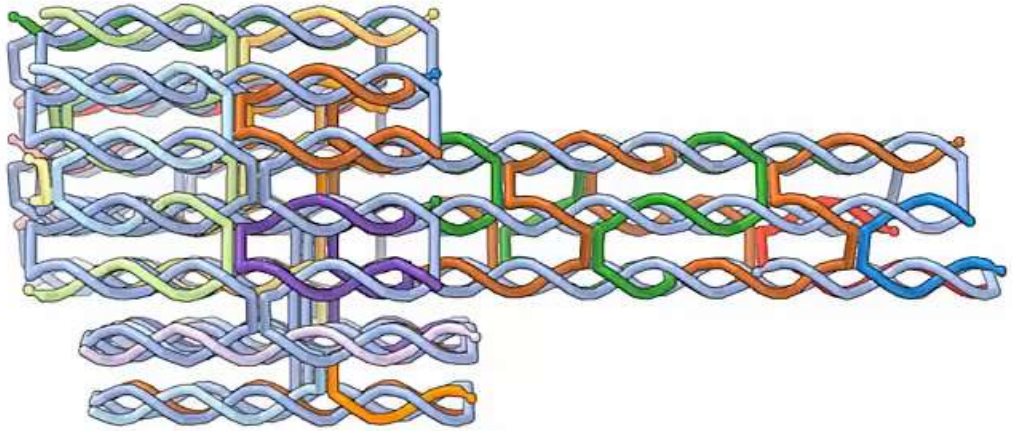
# DimSUM – Interaction Panel



# DimSUM – Interaction Panel

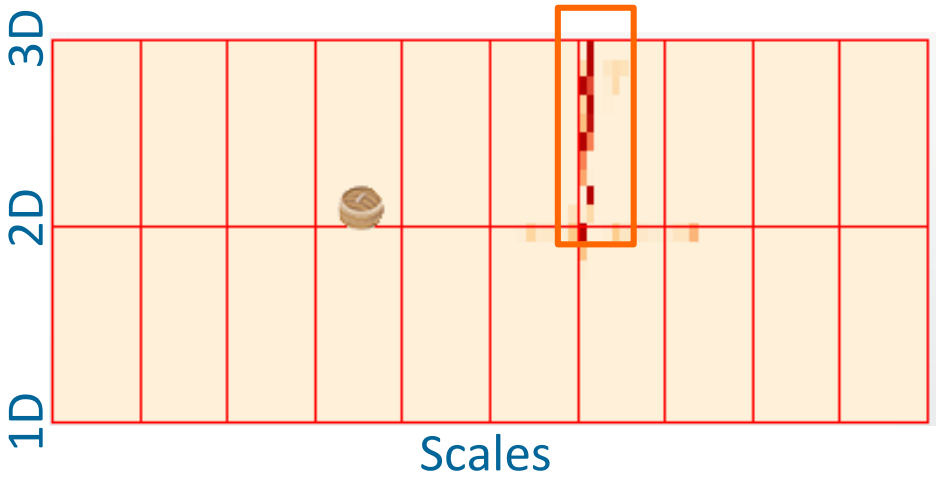


# DimSUM – Interaction Panel

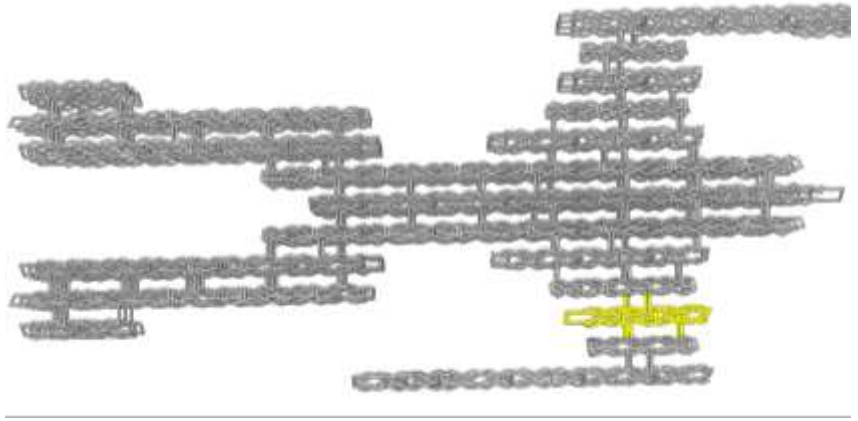



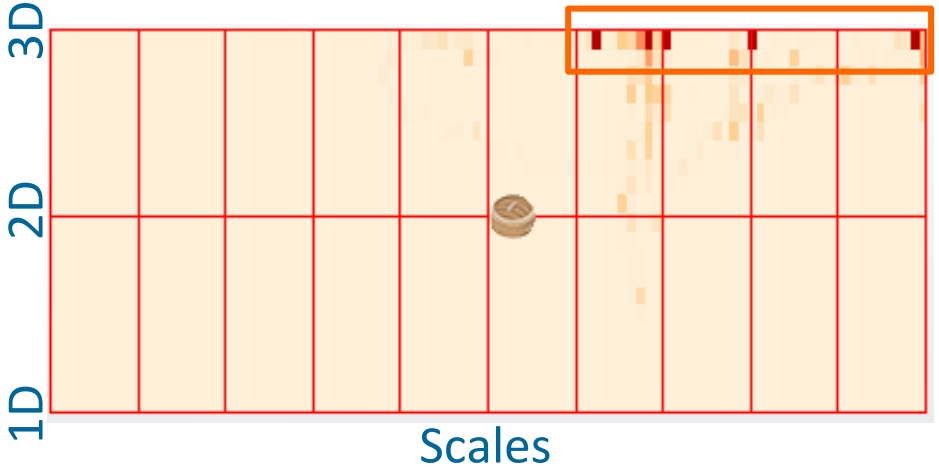
Loading user session

# Case Studies

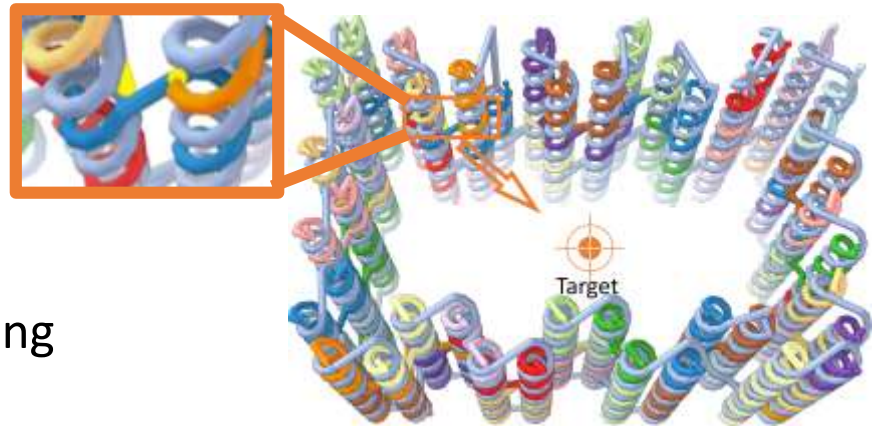



- Case study 1
  - Domain scientist 1
  - Structural motif design
  - Transition 3D to 2D



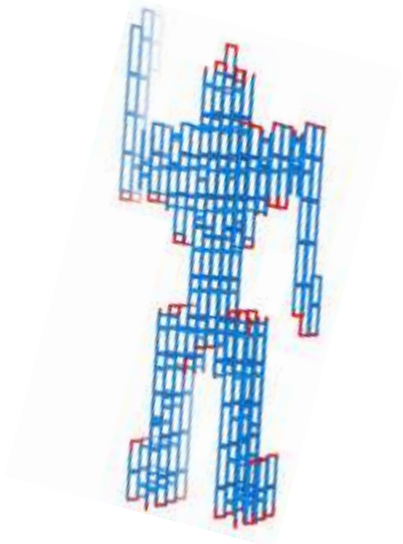



- Case study 2
  - Domain scientist 2
  - Surface strand analysis
  - 3D scales most interesting



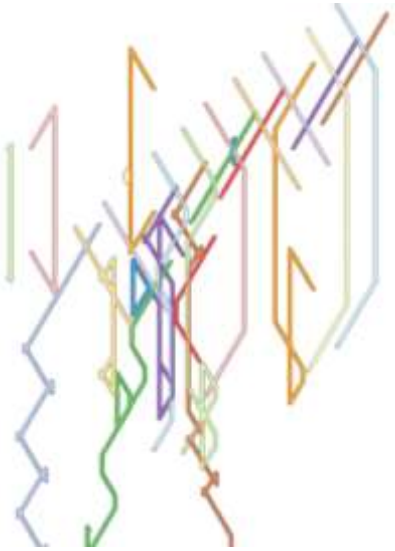
# Limitations & Future Work

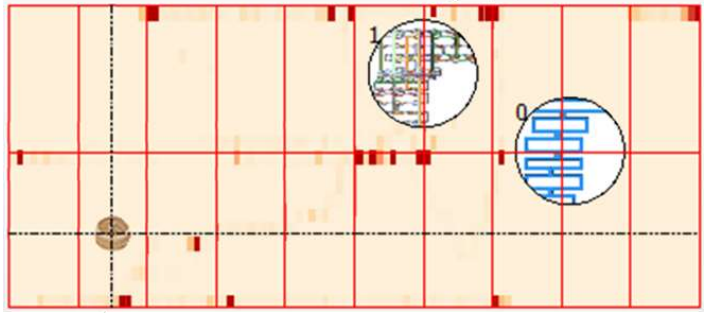
- No simulation data for structural predictions (4D?)
- Camera is not smart (how to keep focus?)
- Transitions from 2D to 1D (two-step interpolation?)
- Navigation in DimSUM panel not guided (guided navigation?)



Our approach

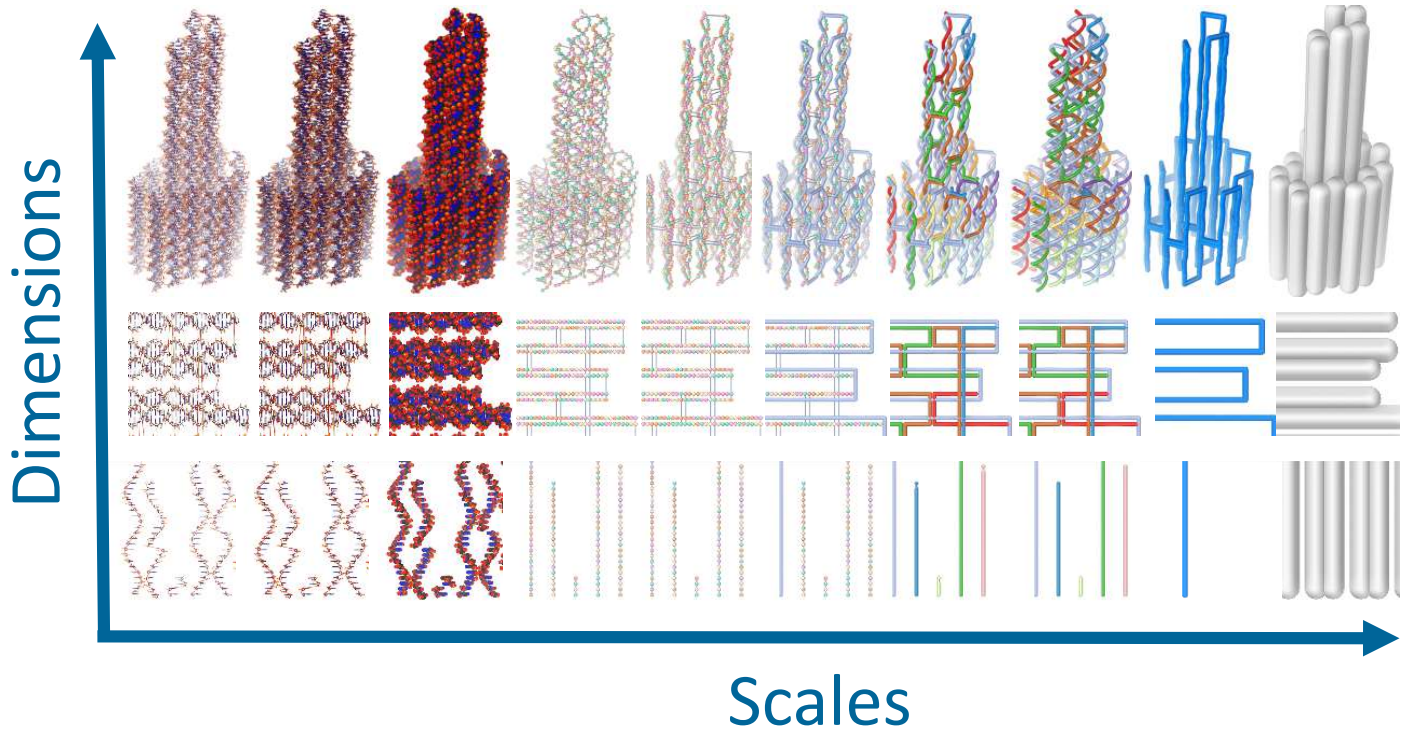

Castro et al. 2011



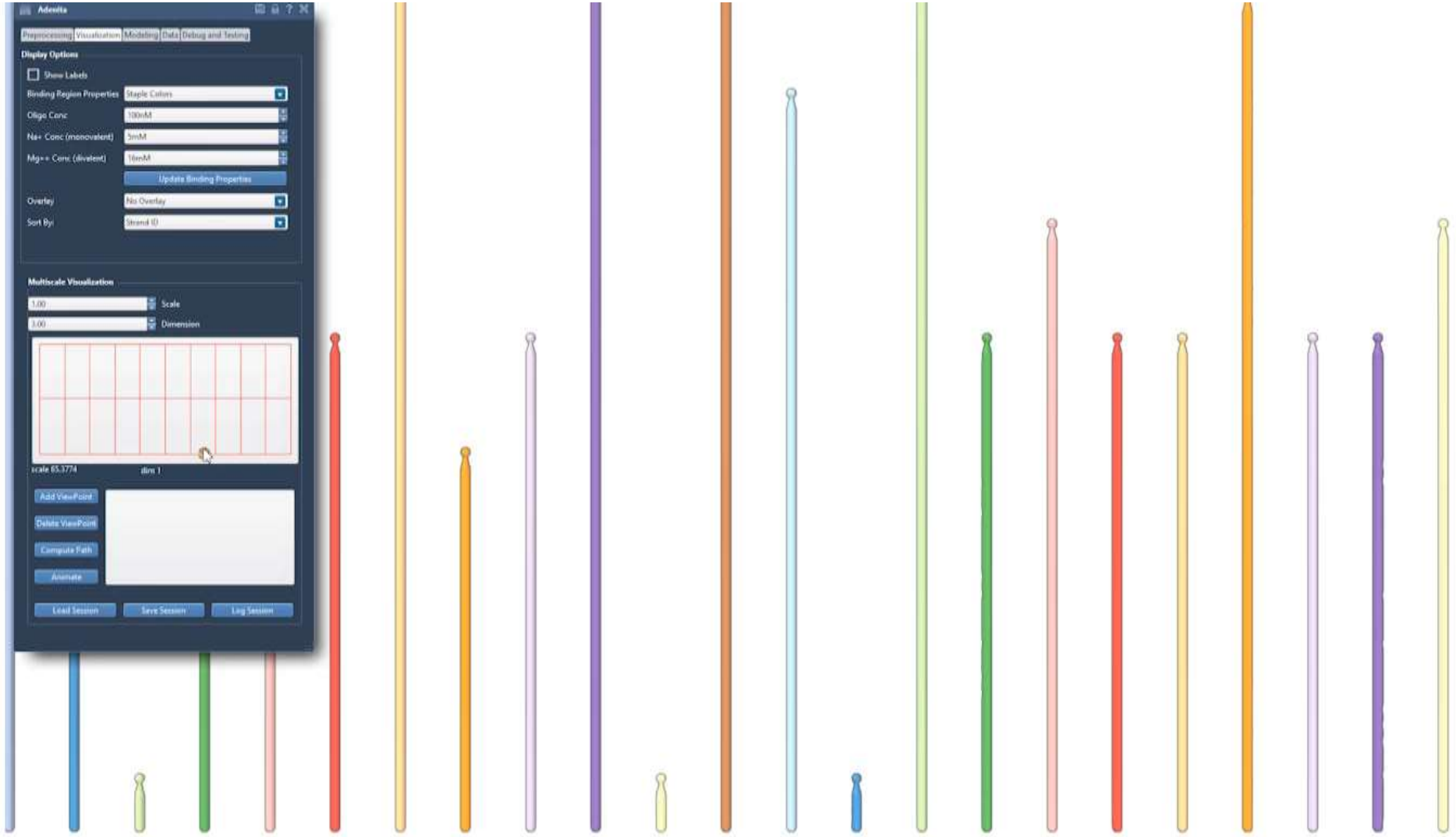


# Summary

- Novel and existing representations for DNA origami structures
- Using visual abstraction
- Integration into a dimension and scale unifying map
- Interaction techniques for exploring the DimSUM
- Abstraction-adaptive modification



# Thank you for your attention!




FWF
Der Wissenschaftsfonds.

M RA

HORIZON 2020