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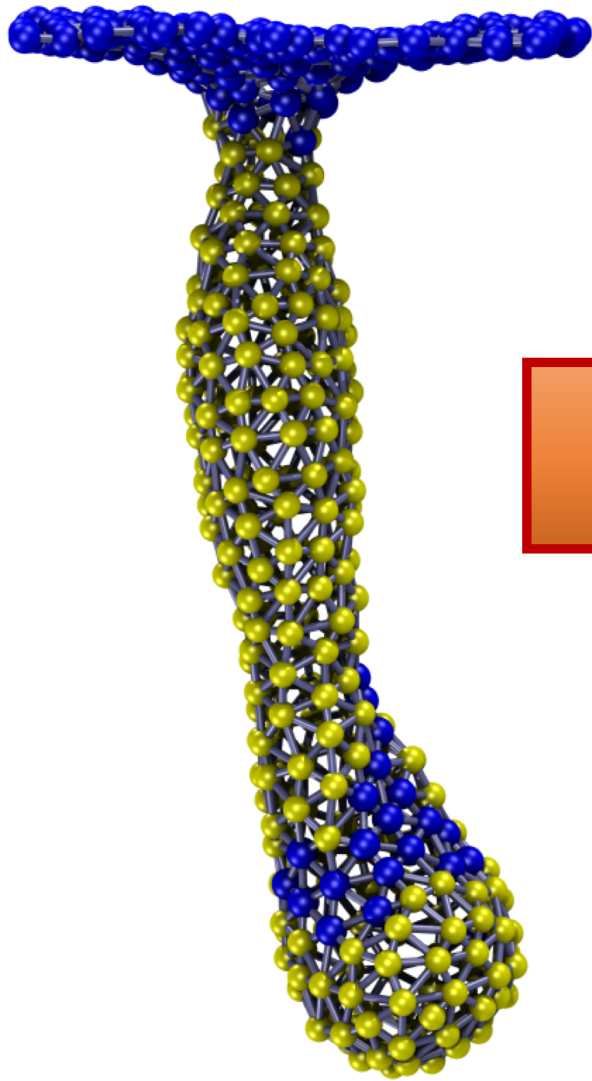
**Martini3 Workshop
2021**

Weria Pezeshkian

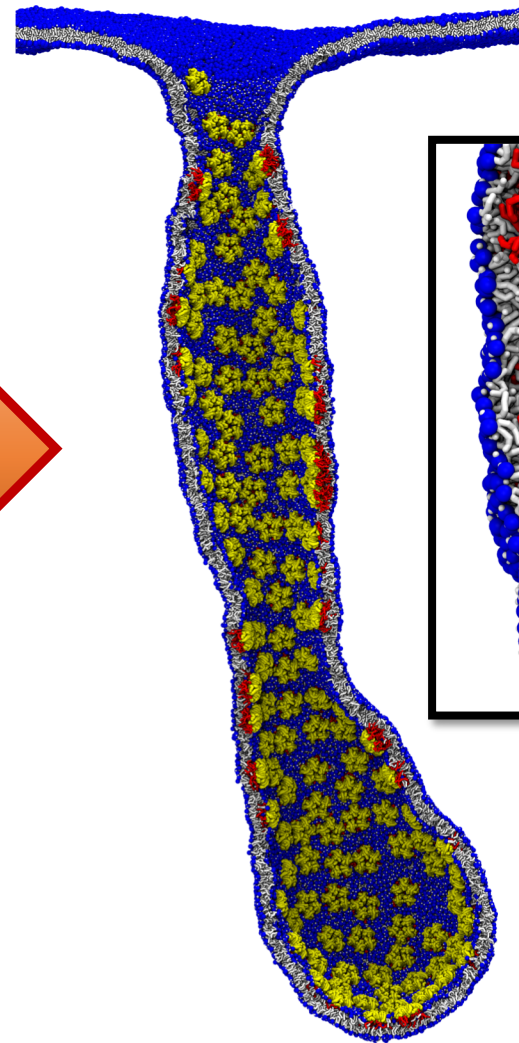
TS2CG

Converting triangulated surfaces to coarse grained membrane model

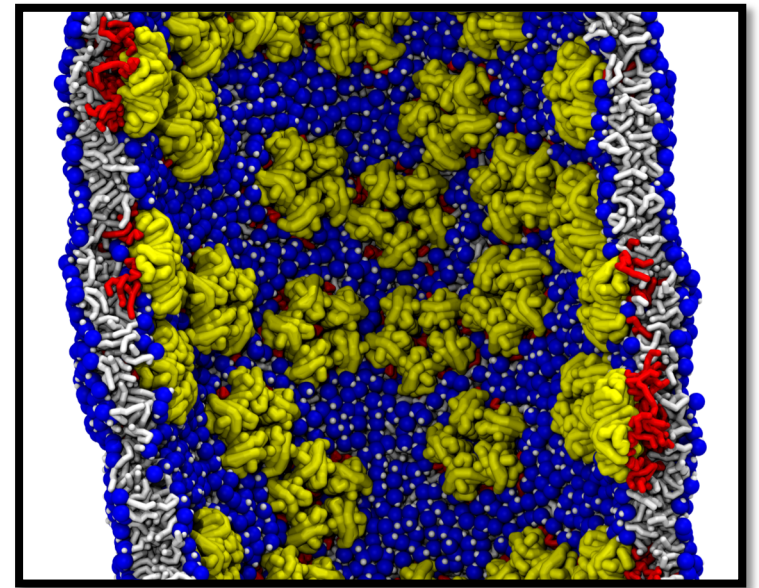
DTS

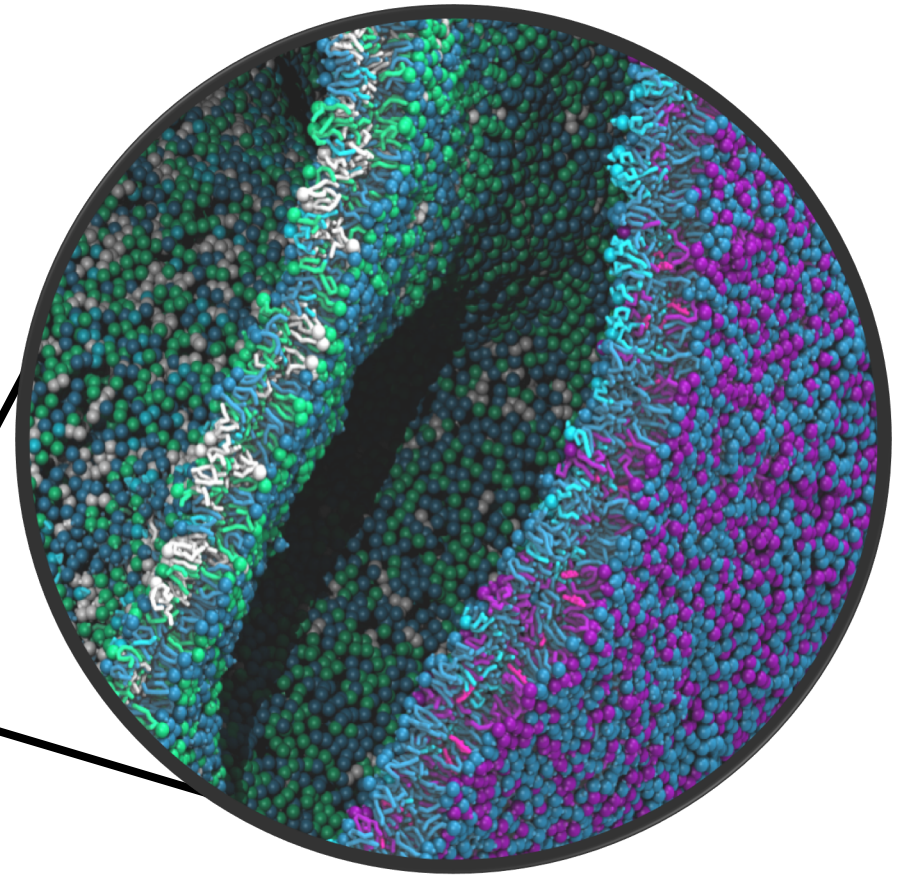
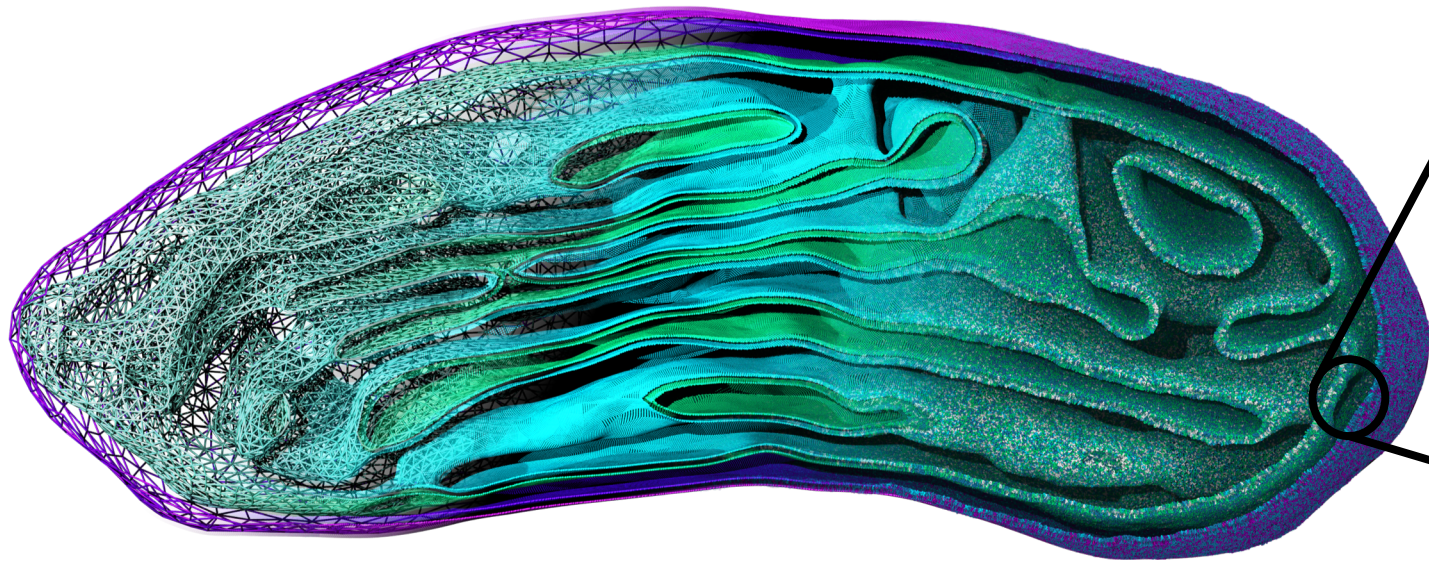


CG

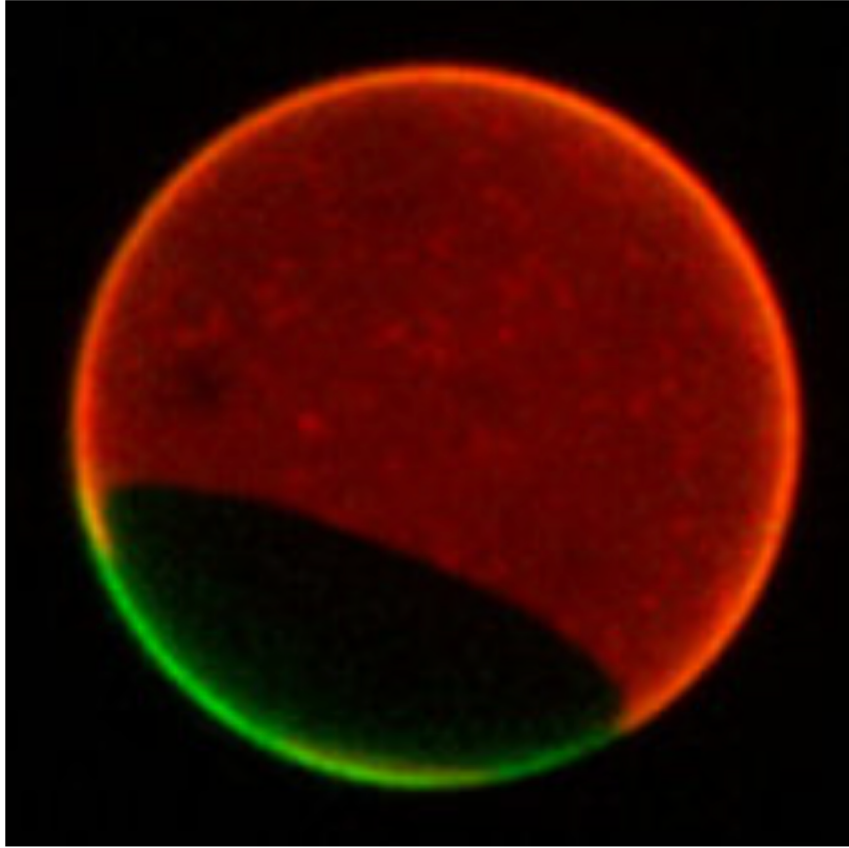


TS2CG

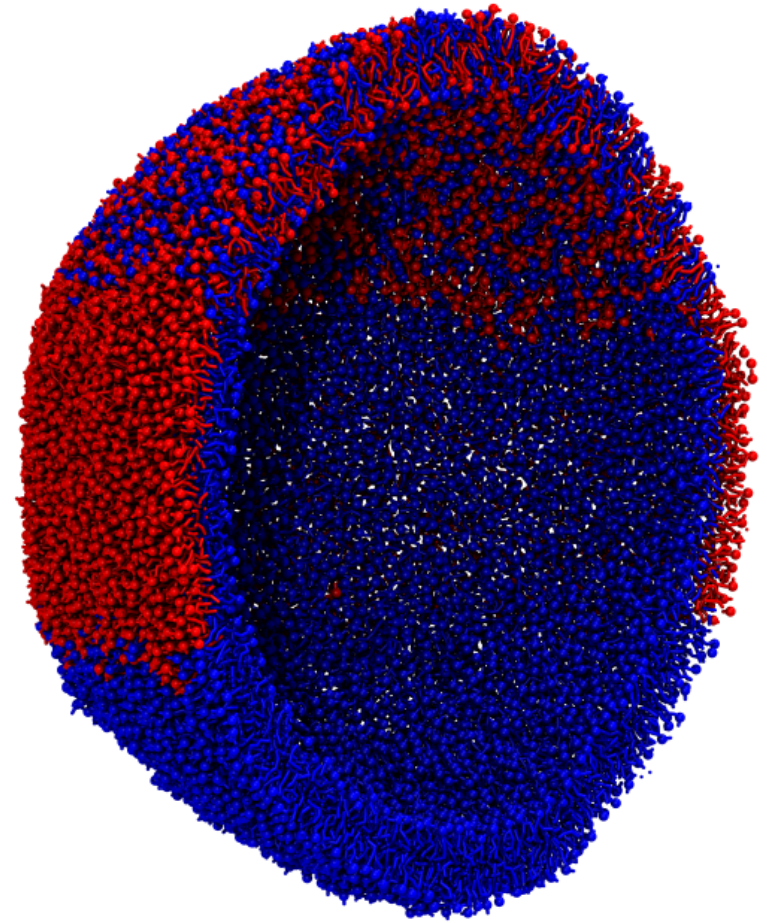




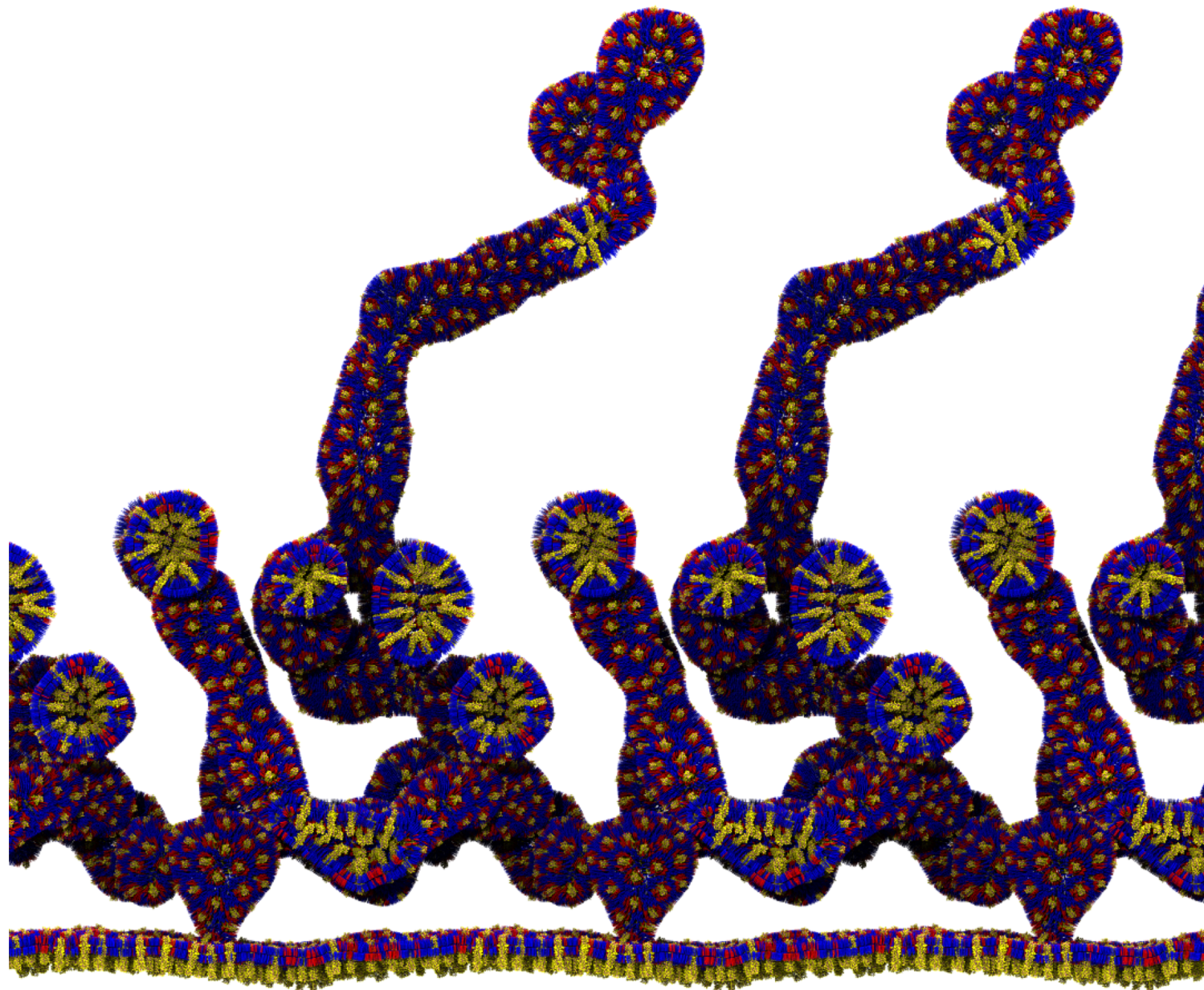
Electron Tomography CG



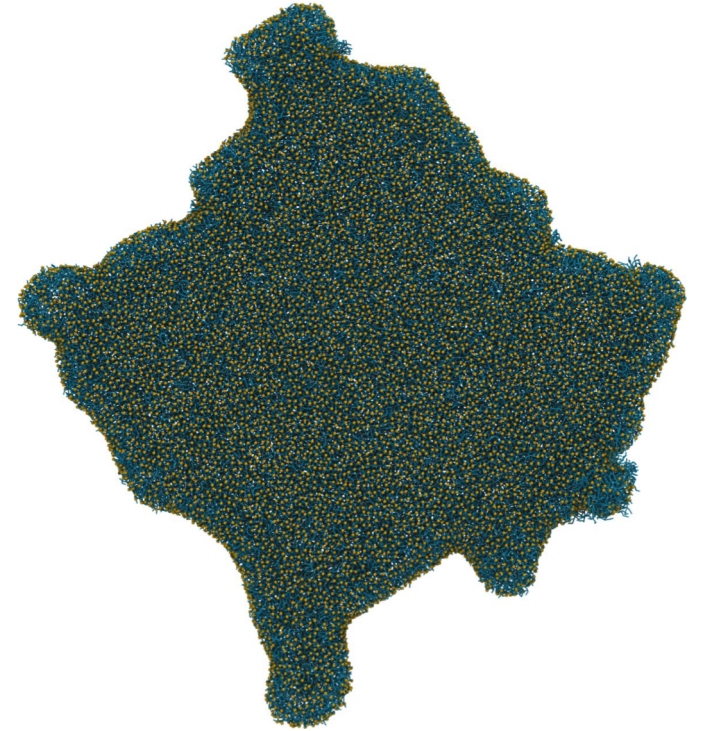
fluorescence microscopy

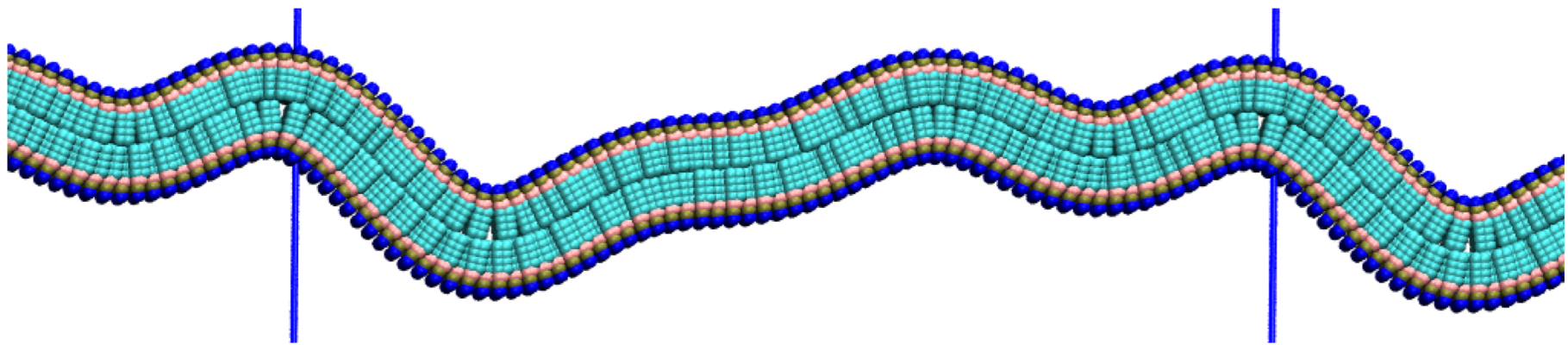


CG

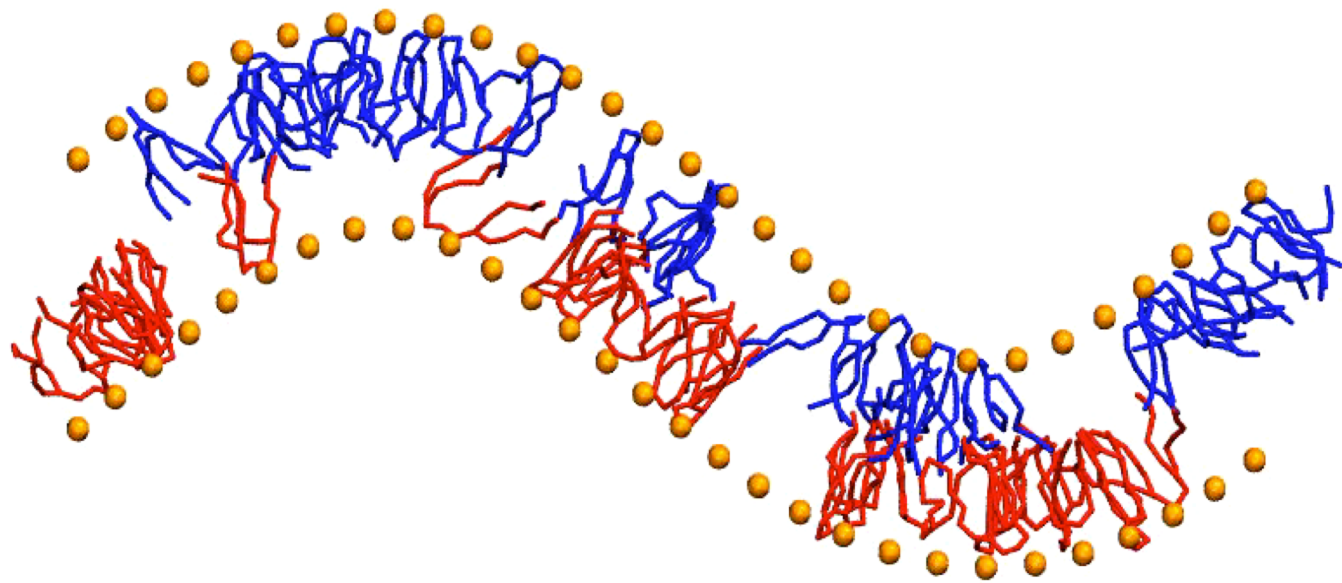


More fun





$$z = \sum_{m,n=1} A_{n,m} \left\{ \sin \left[\frac{2\pi n}{L_x} x + \frac{2\pi m}{L_y} y \right] + \cos \left[\frac{2\pi n}{L_x} x + \frac{2\pi m}{L_y} y \right] \right\}$$



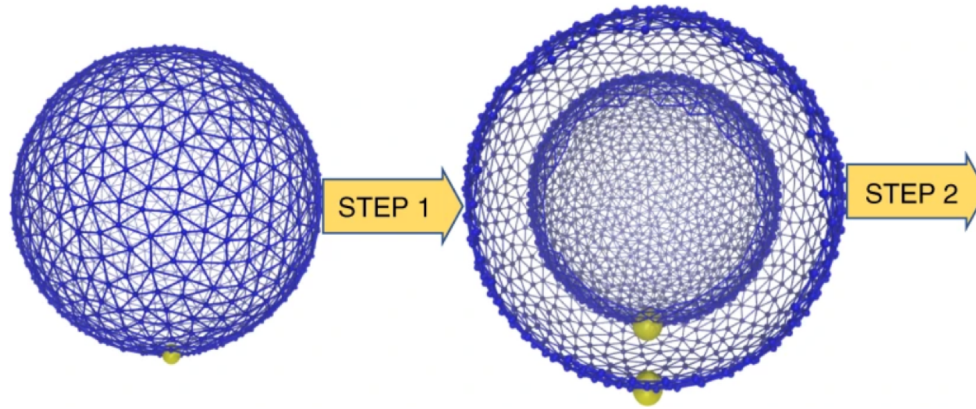
TS2CG Scheme

TS2CG

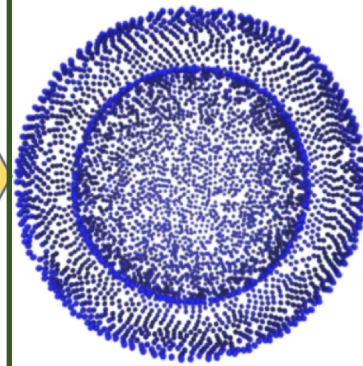
Pointillism

Membrane builder

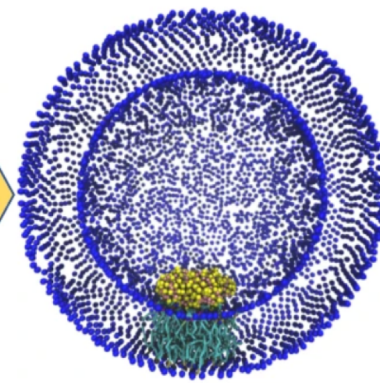
Pointillism



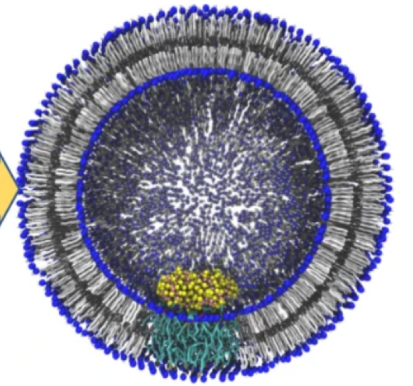
STEP 2



STEP 3



STEP 4



Download and Install

marrink-lab / TS2CG1.1

<> Code

Issues

Pull requests

Actions

Projects

master

TS2CG1.1 / src /

Download latest version at:

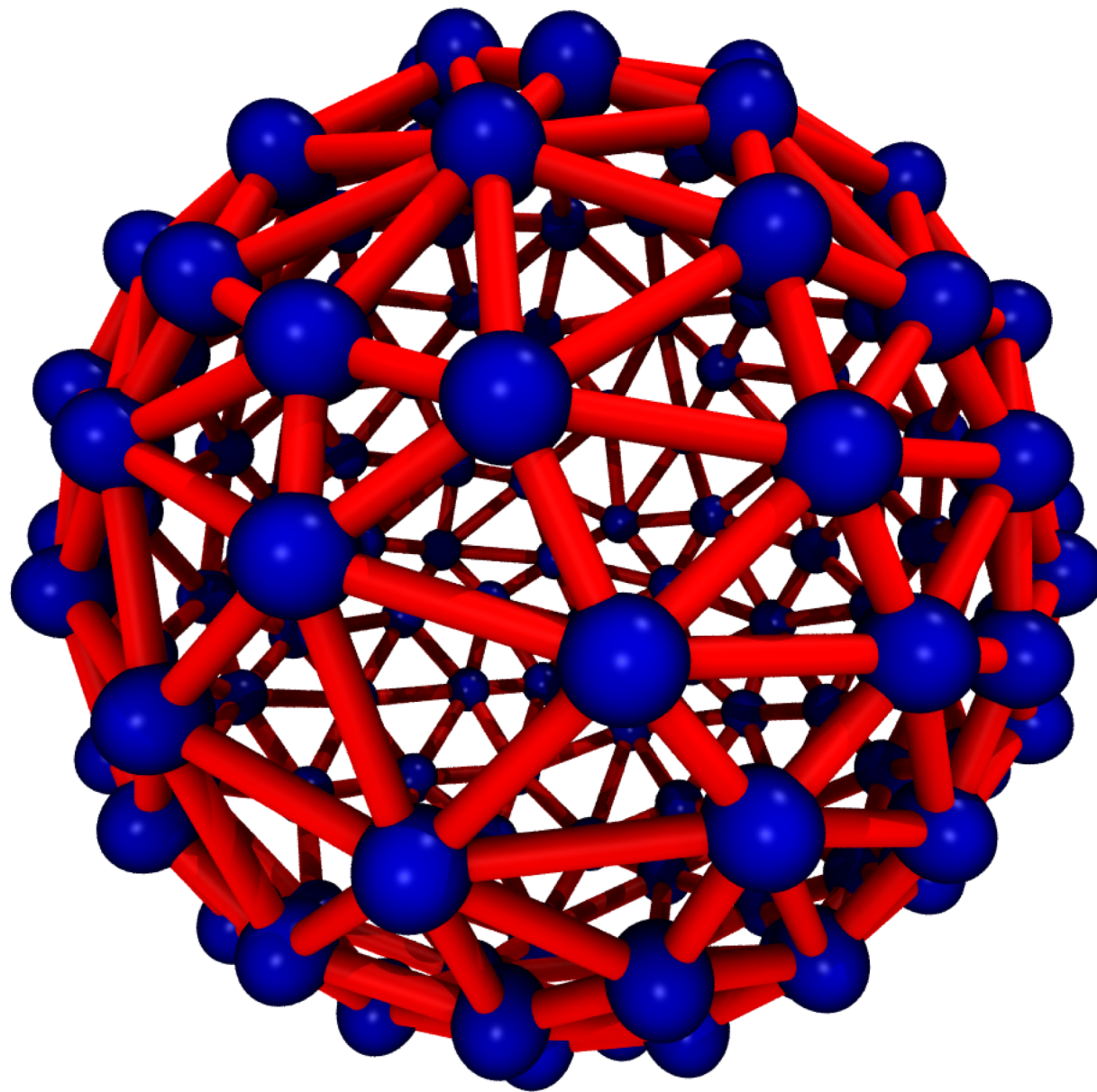
[HTTPs://github.com/marrink-lab/TS2CG1.1](https://github.com/marrink-lab/TS2CG1.1)

```
Werias-MacBook-Pro:TS2CG1.1 weriapezeshkian$ ./compile.sh
```

```
Werias-MacBook-Pro:TS2CG1.1 weriapezeshkian$ ls
PCG                               PyMOL2q.py                       SOL
PLM                               README.md                         Tutorials
```

How to Use TS2CG

**Building a membrane from a
Triangulated Surface**





PCG: Point to CG model

PLM output folder

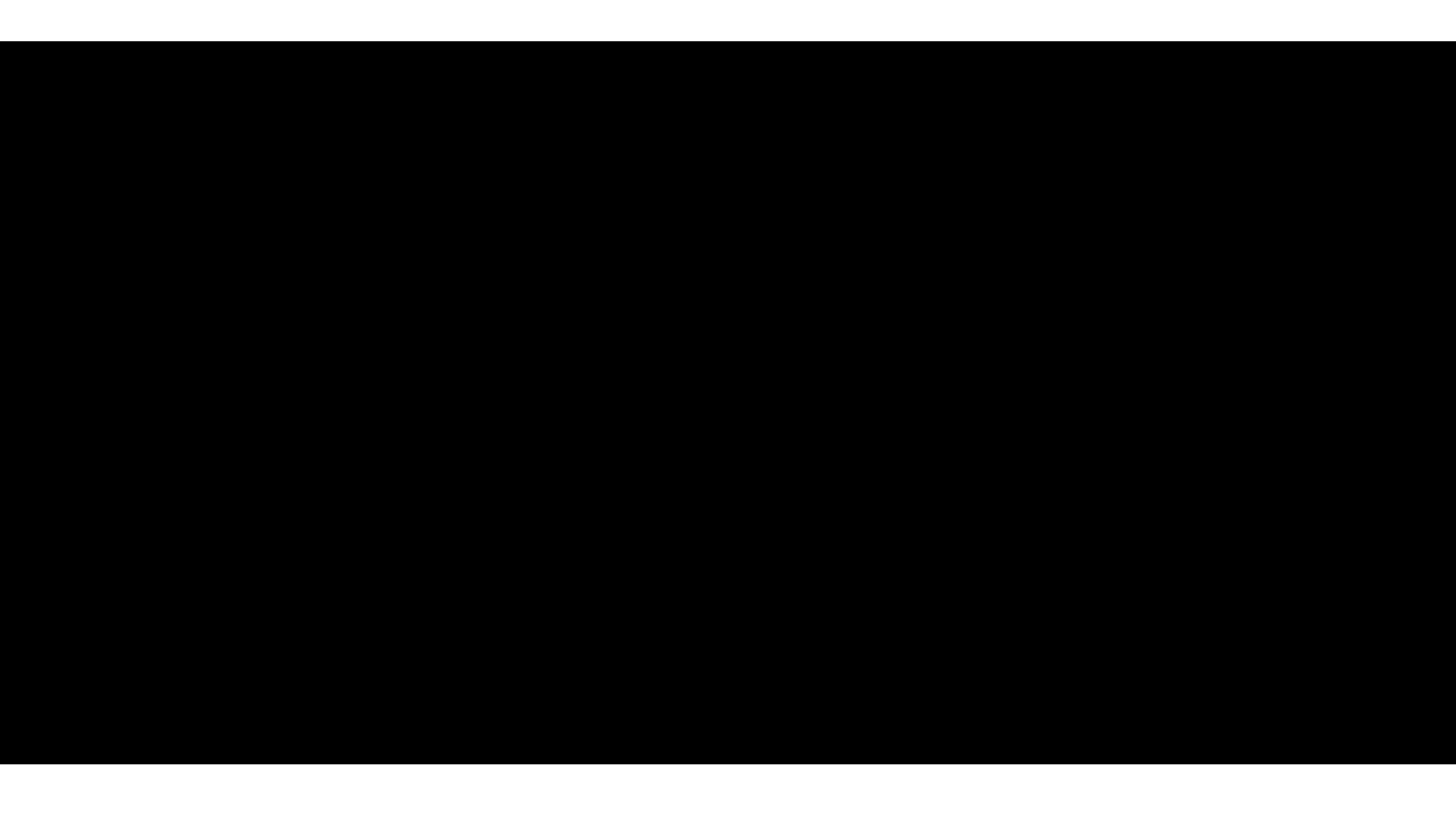
Point: no extension

Lipid structure file:

Martini3.LIB: LIB extension

System composition file:

Input.str: str extension



File Format

Molecule structure file (must have LIB extension)

```
Description Martini Map CG
```

```
Version Martini3
```

```
[ DOPC ]
```

```
1 NC3 0 0 1  
2 PO4 0 0 0  
3 GL1 0 0 -1  
4 GL2 0 0.5 -1  
5 C1A 0 0 -2  
6 D2A 0 0 -3  
7 C3A 0 a -4  
8 C4A 0 0 -5  
9 C1B 0 1 -2  
10 C2B 0 1 -3  
11 C3B 0 1 -4  
12 C4B 0 1 -5
```

System composition file (must have str extension)

```
include P1.gro  
include P2.gro
```

```
[Lipids List]
```

```
Domain 0
```

```
POPC 0.6 0.4 0.65
```

```
DOPC 0.4 0.6 0.67
```

```
End
```

```
Domain 1
```

```
DPPC 0.5 0.5 0.55
```

```
CHOL 0.5 0.5 0.40
```

```
End
```

```
[Protein List]
```

```
protein1 1 0.01 0 0 3.7
```

```
protein2 2 0.01 0 0 -2.4
```

```
End Protein
```

TS file: tsi file format

```
version 1.1
```

```
box      50.0      50.00      50.0
```

```
vertex      130  
0      21.16      25.43      25.59      0  
1      27.02      23.20      21.67      0  
2      26.99      25.51      28.01      1
```

```
triangle     256  
0 11 55 43  
1 94 75 14  
2 64 3 91
```

```
inclusion      2  
0 1 22      0 1  
1 1 5      0 1
```

composition file

```
include P1.gro  
include P2.gro
```

```
[Lipids List]  
Domain 0  
POPC 0.5 0.5 0.65  
DOPC 0.5 0.5 0.67  
End  
Domain 1  
DPPC 0.5 0.5 0.55  
CHOL 0.5 0.5 0.40  
End
```

```
[Protein List]  
protein1 1 0.01 0 0 -3.7  
protein2 2 0.01 0 0 -2.4  
End Protein
```

TS file: tsi file format

```
version 1.1
```

```
box      50.0      50.00      50.0
```

```
vertex    130
  0      21.16      25.43      25.59      1
  1      27.02      23.20      21.67      1
  2      26.99      25.51      28.01      0
```

```
triangle  256
  0  11  55  43
  1  94  75  14
  2  64   3  91
```

```
inclusion   2
  0  1  22  0  1
  1  1   5  0  1
```

composition file

```
include P1.gro
include P2.gro
```

```
[Lipids List]
Domain 0
POPC 0.5 0.5 0.65
DOPC 0.5 0.5 0.67
End
Domain 1
DPPC 0.5 0.5 0.55
CHOL 0.5 0.5 0.40
End
```

```
[Protein List]
protein1 1 0.01 0 0 -3.7
protein2 2 0.01 0 0 -2.4
End Protein
```

For more information



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@WPezeshkian

Cite: W. Pezeshkian et al, Nature Communications **11**, 2296

