



KØBENHAVNS  
UNIVERSITET

# TS2CG

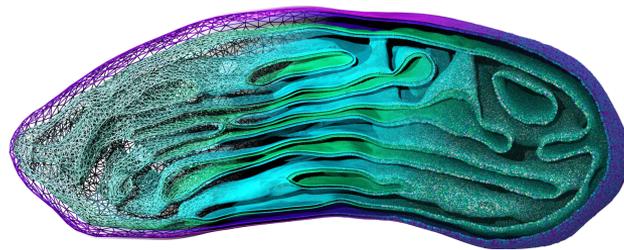
**Backmapping tool or input builder?**

Weria Pezeshkian

August 2025

Groningen, Netherlands

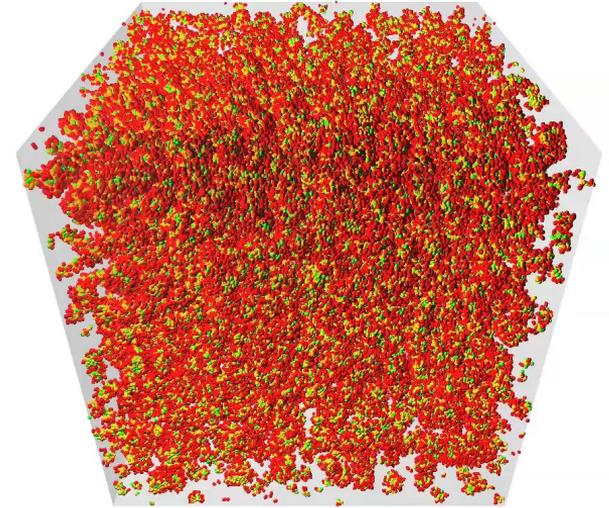
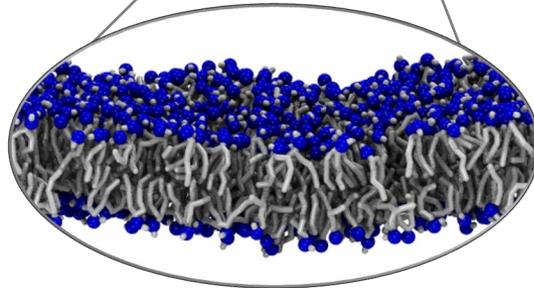
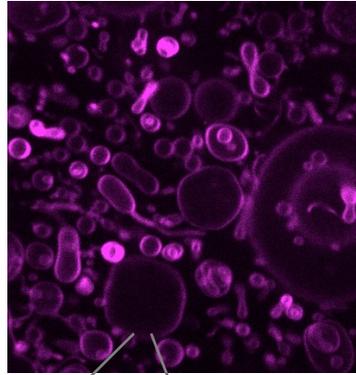
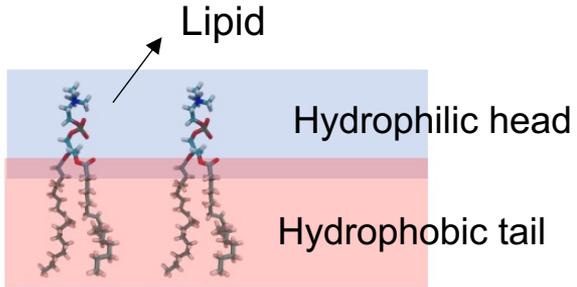
Martini workshop 2025



<https://commicgroup.ku.dk>

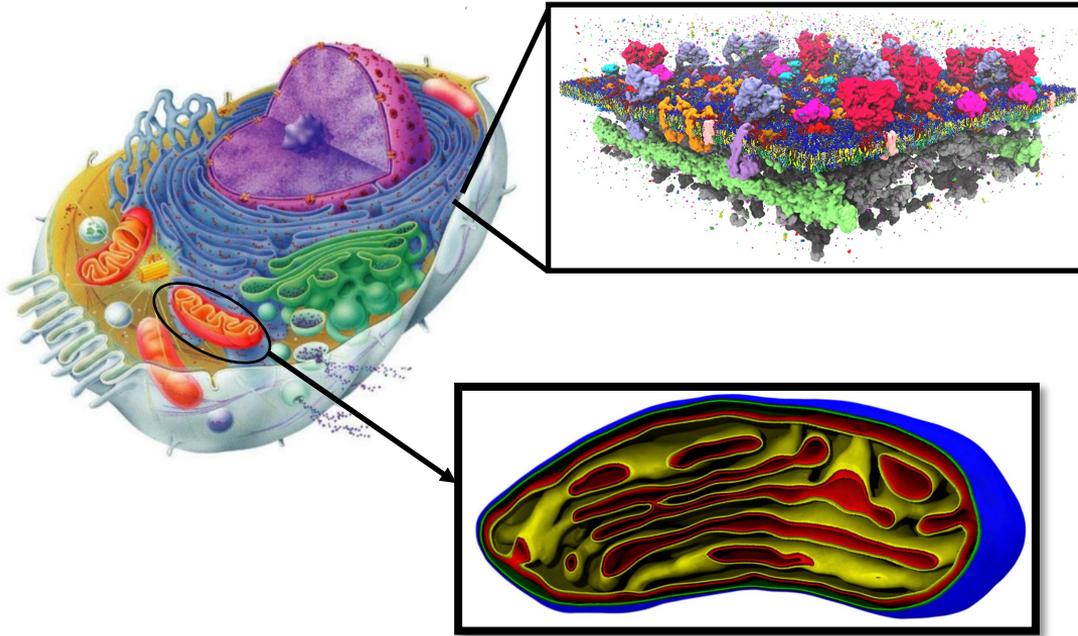
# Lipid bilayers

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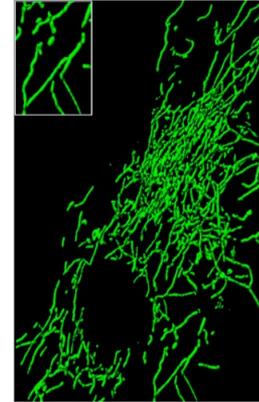


# Biomembranes

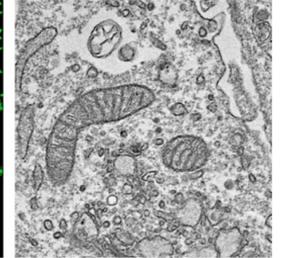
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cellular scale



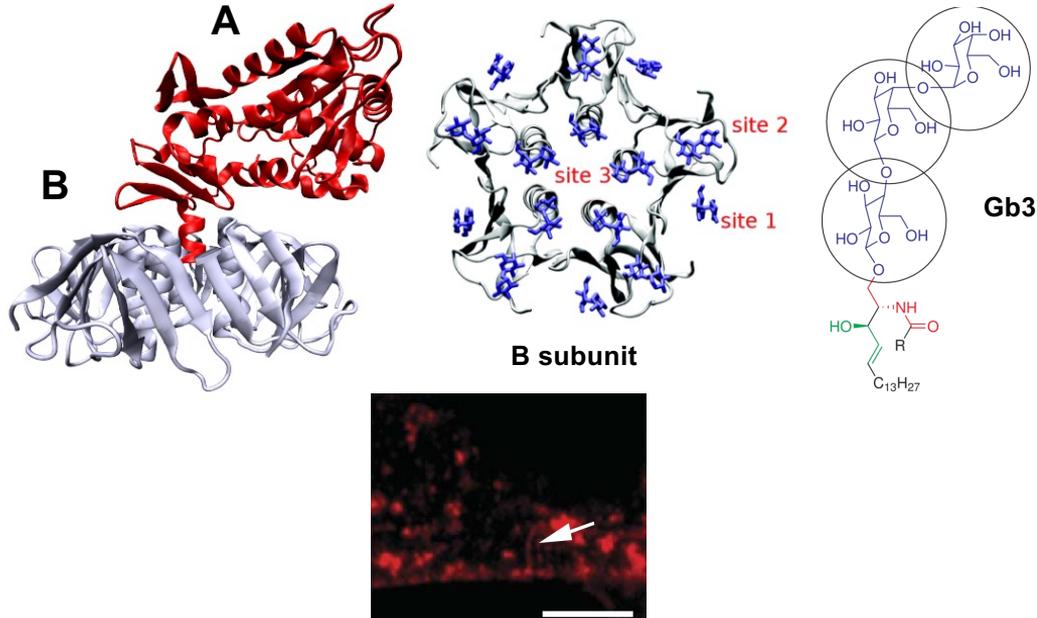
ultrastructure



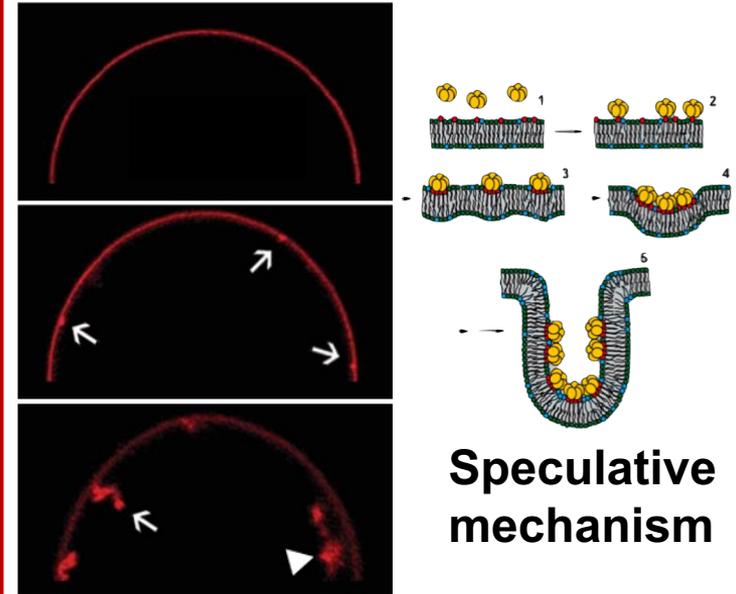
multiscale shape organization of mitochondria

# Initial stage of Shiga toxin internalization

Shiga toxin creates its own route to enter the cell



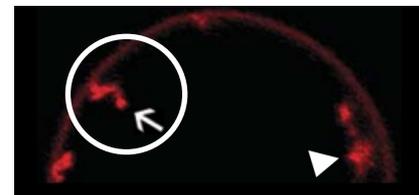
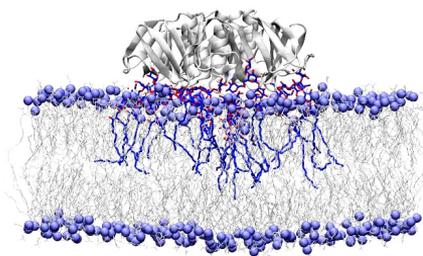
without the complexity of the cell



all-atom

Coarse-grained

mesoscale



Scale

# Commercial break

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Skip after three slides

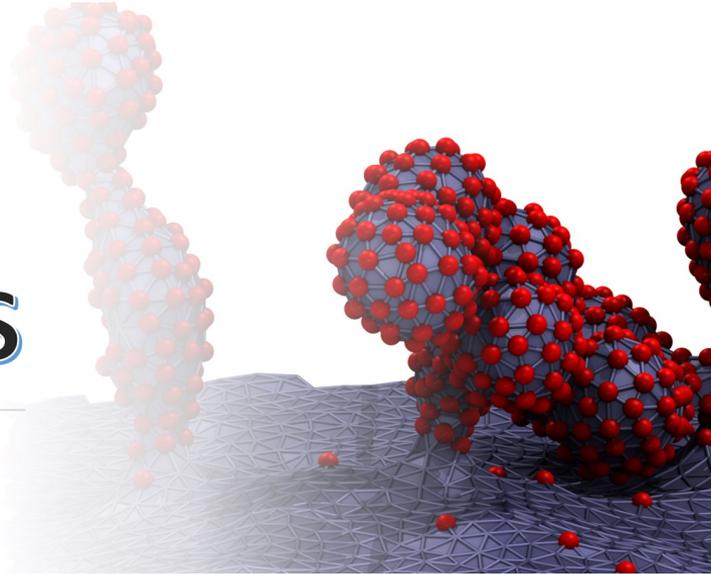
# Mesoscale modeling of biomembranes

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**FreeDTS**

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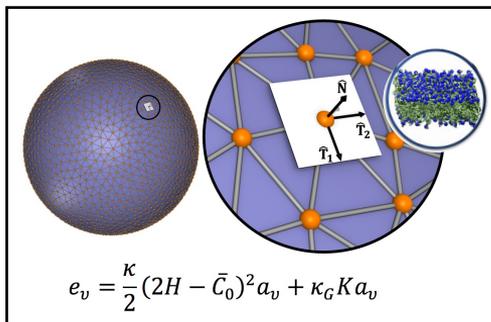


<https://github.com/weria-pezeskian/FreeDTS/>

Pezeshkian et. al. Nat. Commun. (2024)

# FreeDTS Force field

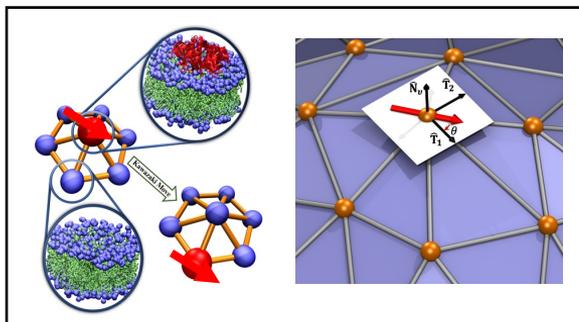
Membrane



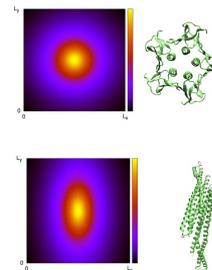
Membrane FF

$$[\kappa, \kappa_G, \bar{C}_0]$$

Proteins



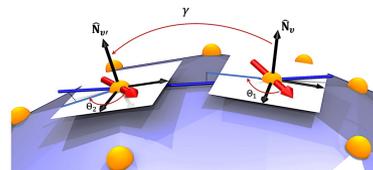
Proteins-Membrane interaction



$$[\bar{C}_0, \Delta\kappa, \Delta\kappa_G]$$

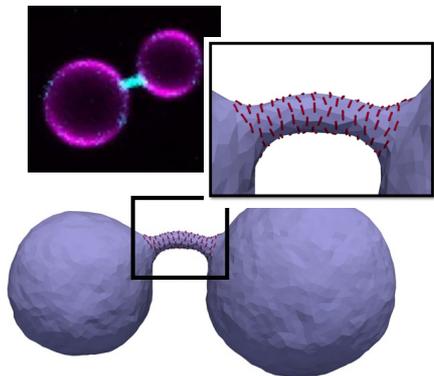
$$[k_{\parallel}, C_0^{\parallel}, k_{\perp}, C_0^{\perp}]$$

Proteins-protein interaction



$$e_{inc,inc} = -A_{i,j} - B_{i,j} \cos[N(\Theta - \Theta_0)] - C_{i,j} \cos[\gamma - \gamma_0]$$

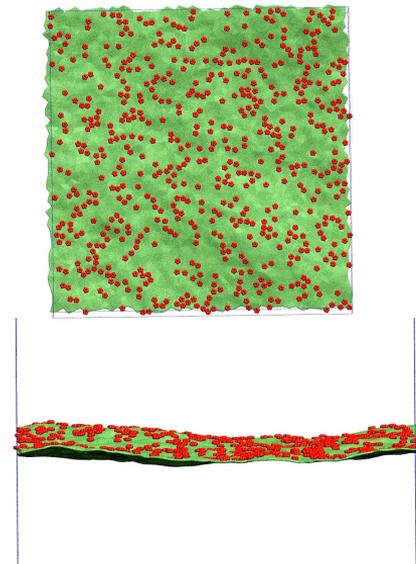
# FreeDTS applications



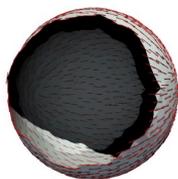
Protein induced neck constriction



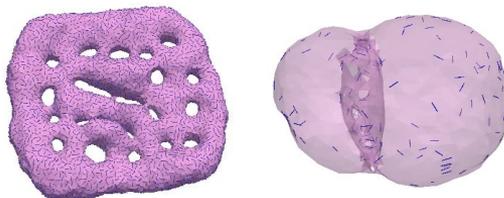
Tube pulling



endocytosis



membrane repair

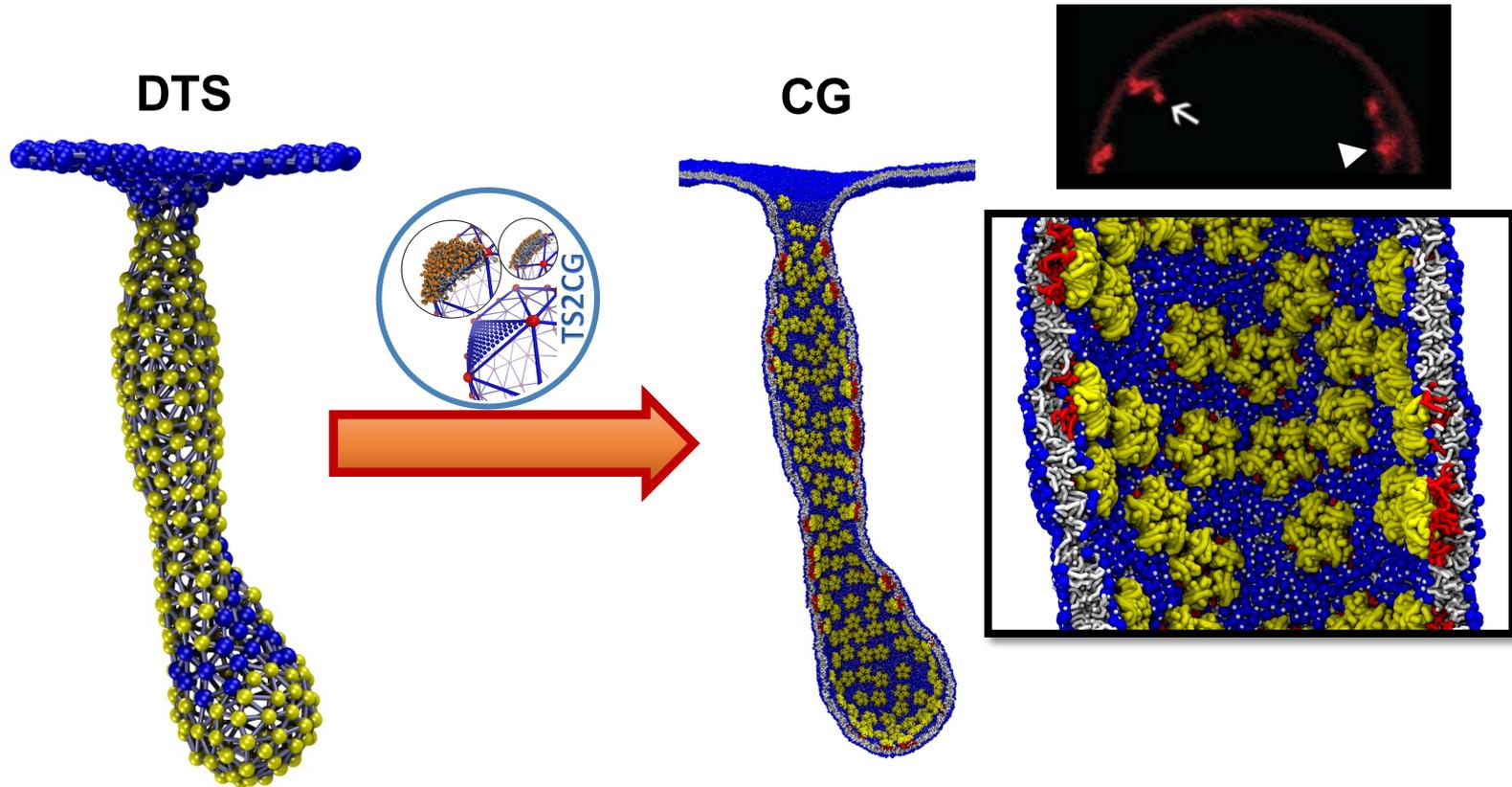


organelle shapes

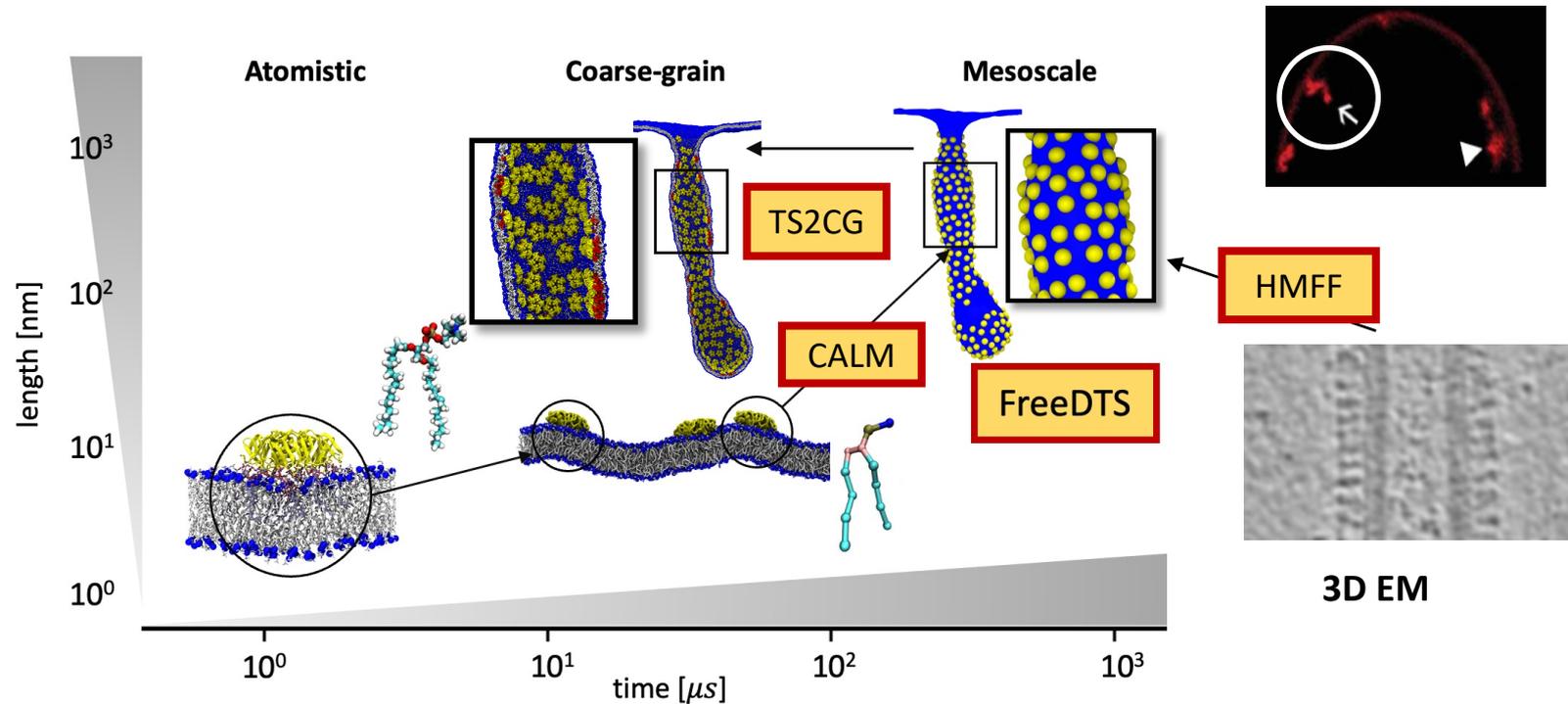
Pezeshkian et. al. Nature Communications (2024)  
Cornet et al, Soft matter, 20, 4998 (2024)  
Pezeshkian et al, Structure 31, 492 (2023)  
De Franceschi et al, ACS Nano 17, 966 (2023)

# Molecular architecture of the tube

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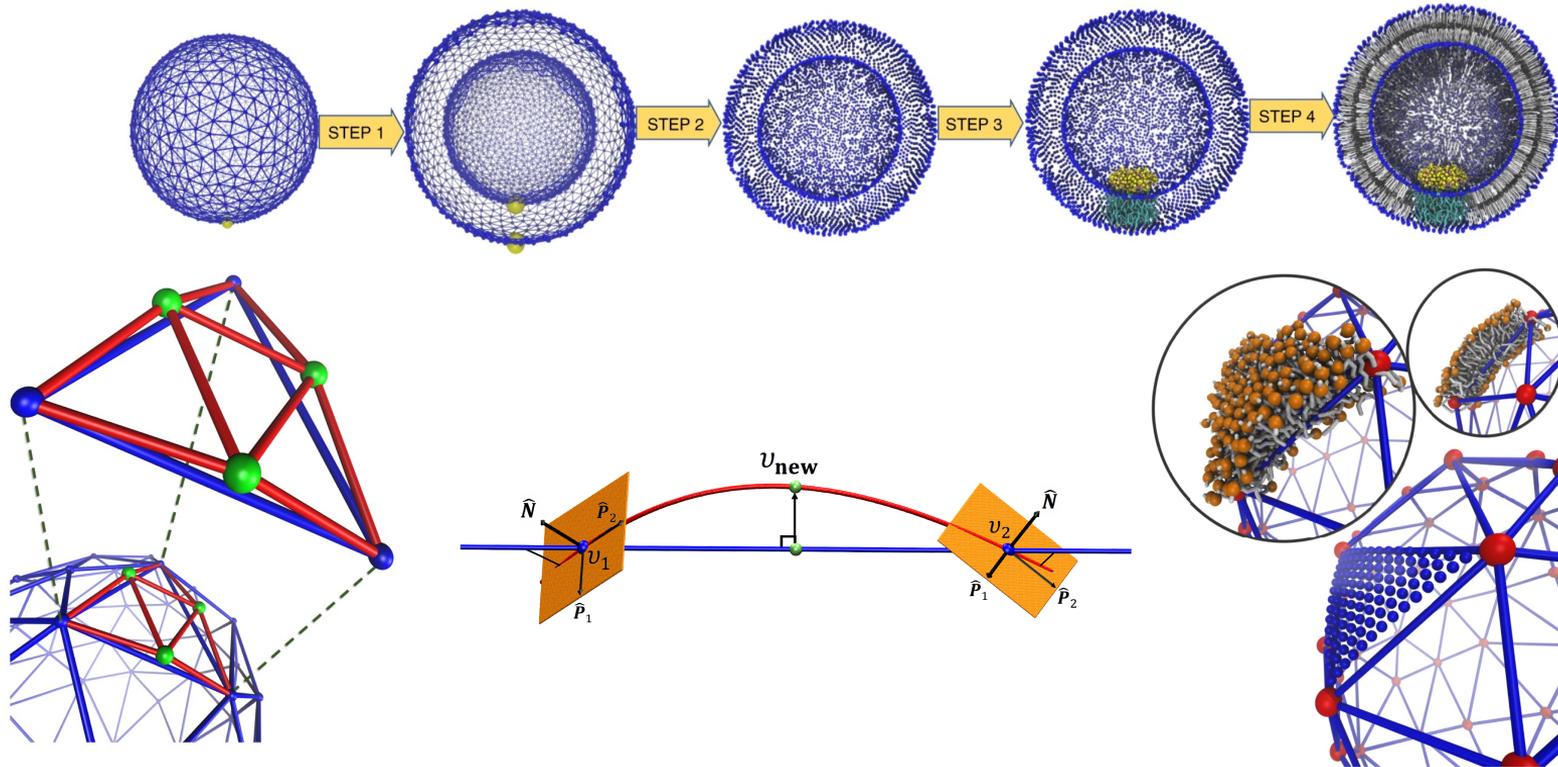


# Multiscale simulation at a glance



Pezeshkian et al, Nat. Commun; (2024), Pezeshkian et al, Nat. Commun; (2020), Pezeshkian et al, Curr. Opin. Cell Biol. (2021), Maurer et al (2025), Schuhmann, Angew. Chem. (2025).

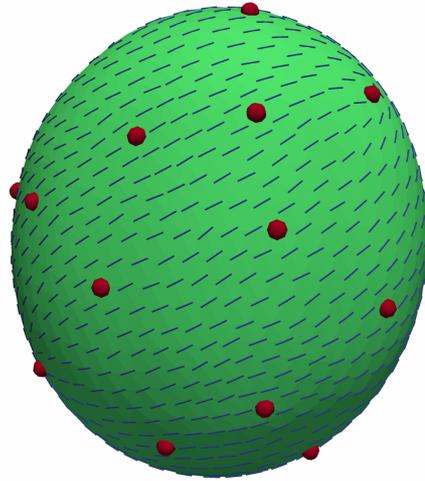
# Basic idea of TS2CG



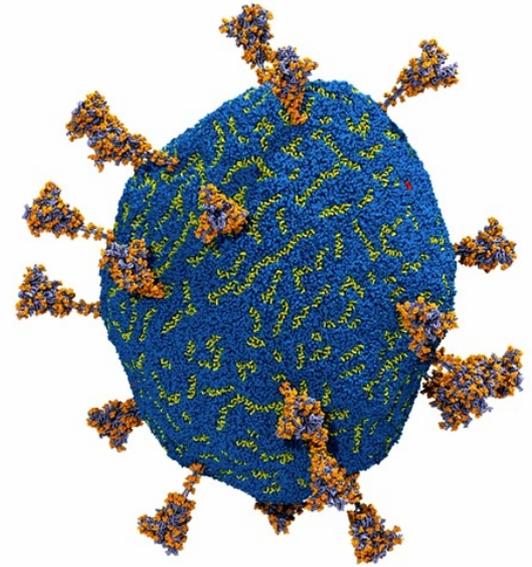
# SARS-CoV-2 envelope

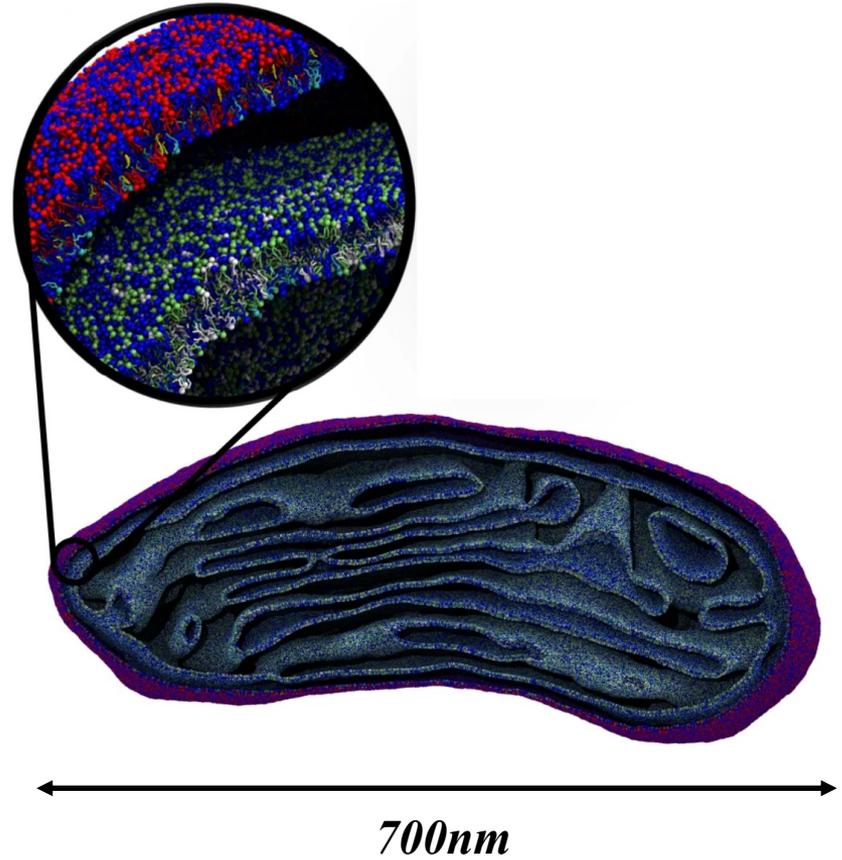
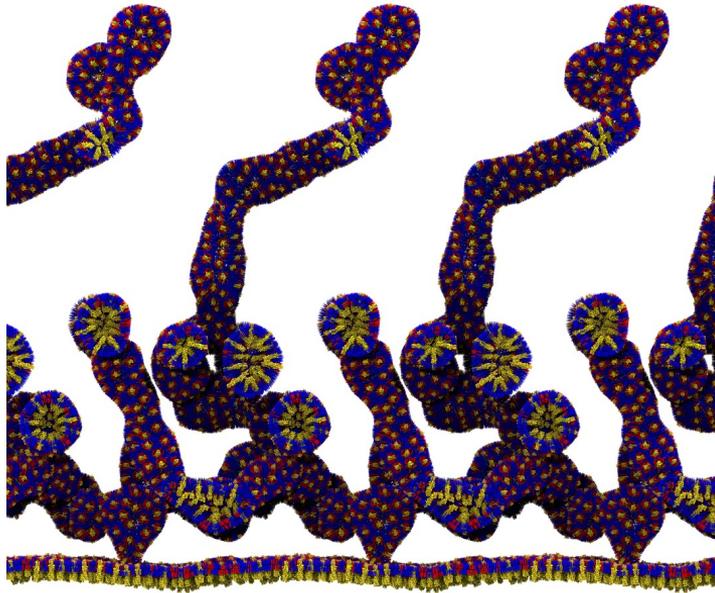
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- Spike protein (25)
- ▮ M dimer (1000)
- E pentamer (3)



TS2CG





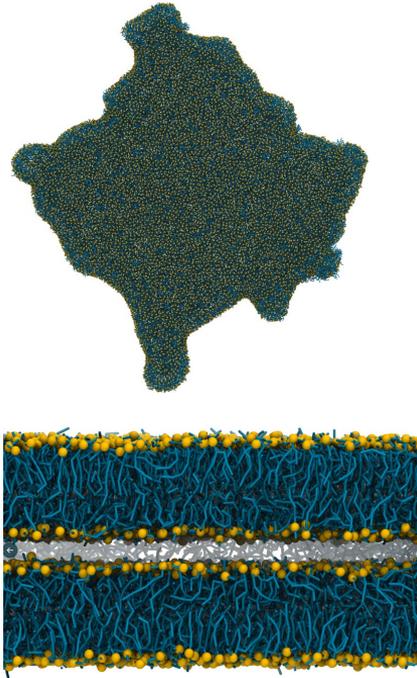
# Martini Exhibition

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Martini bunny



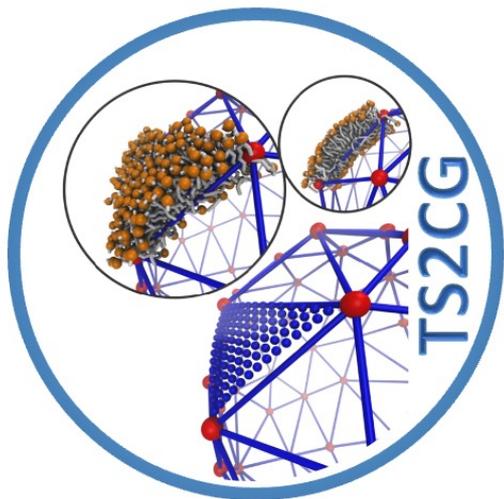
Martini Kosovo



Martini Glass



Credit: Matthieu Chavent and others on Twitter whose names I cannot recall.



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Version 1.x

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C++

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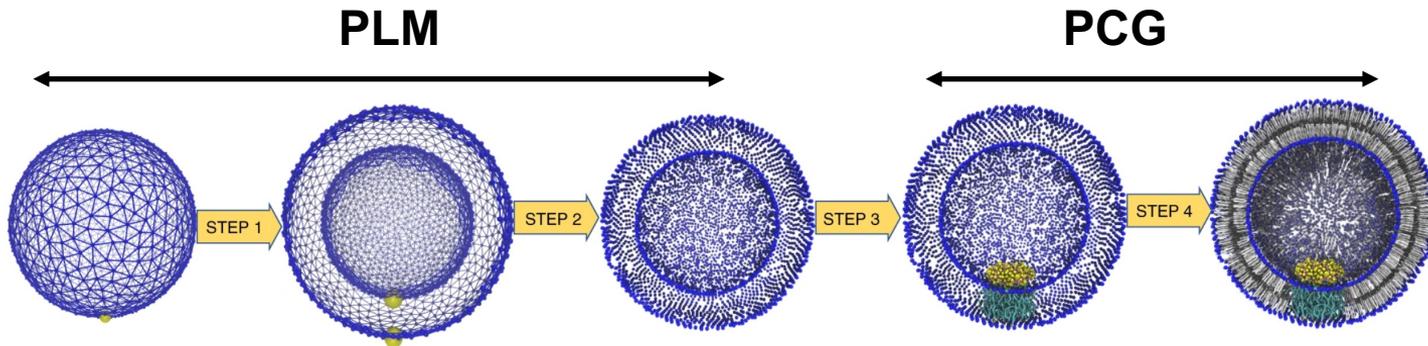
PLM: Pointillism

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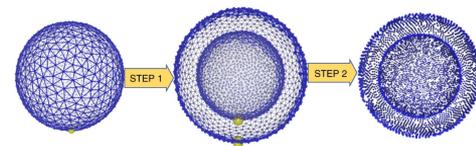
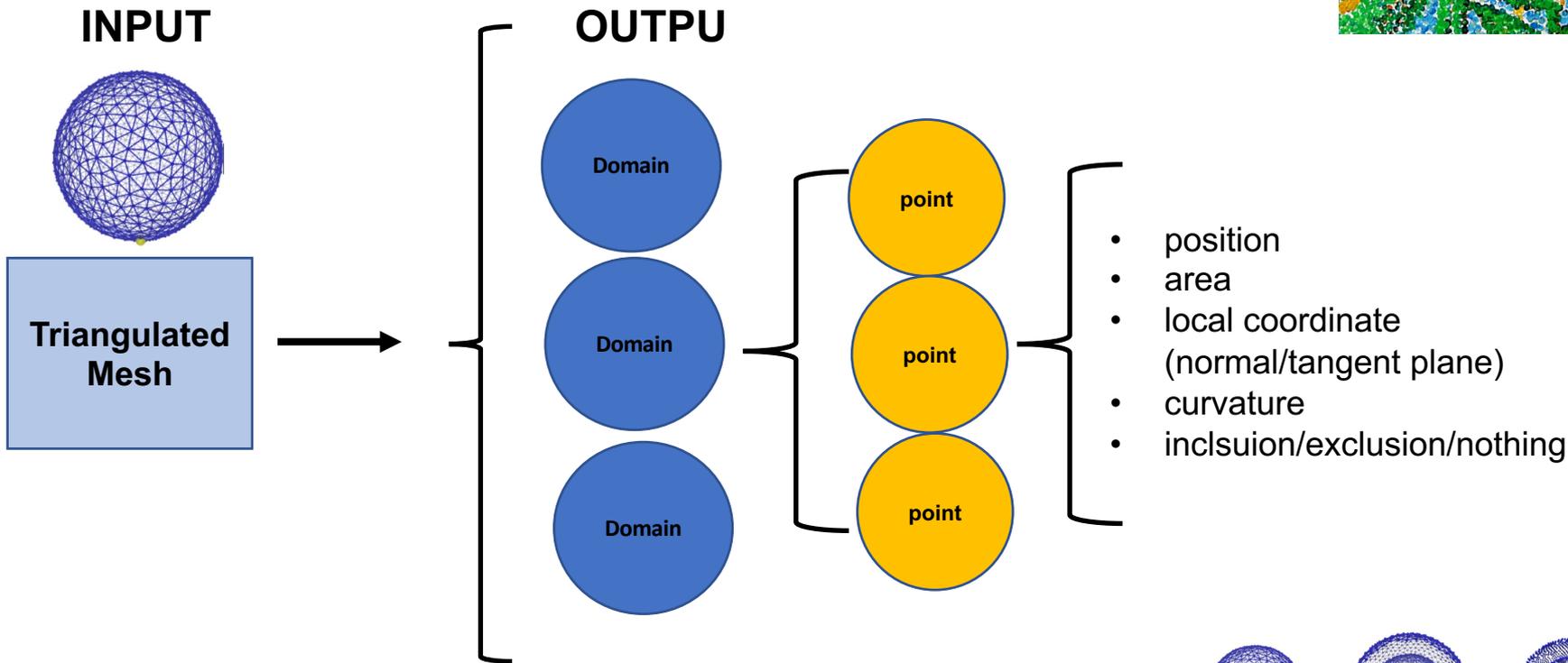
PCG: Point-to-Coarse-Grained Model

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SOL: Fast solvation



# Pointillism: PLM



# Membrane Builder: PCG

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## INPUT

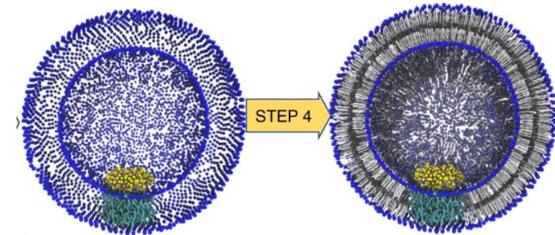
- Lipid composition for each domain.
- A protein structure for each inclusion type.
- Lipid map file

## STEP

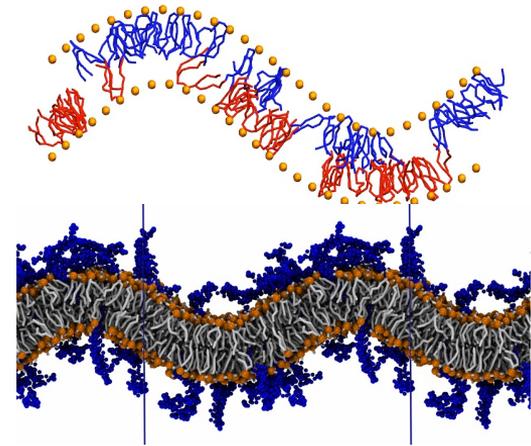
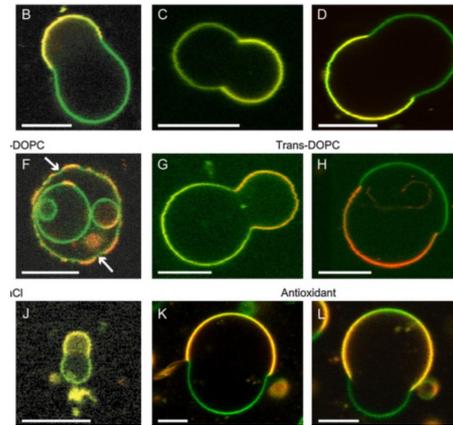
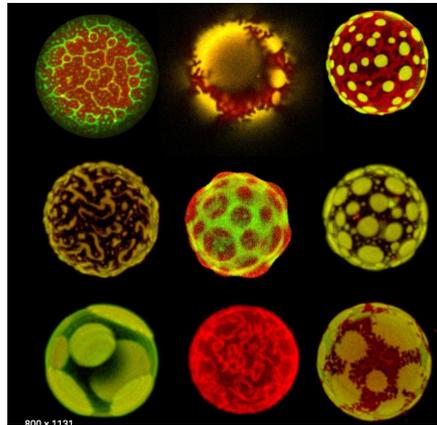
- Place the protein in the inclusion location.
- Remove points within the exclusion zone and those overlapping with proteins.
- Randomly place lipids with the defined composition.

## OUTPUT

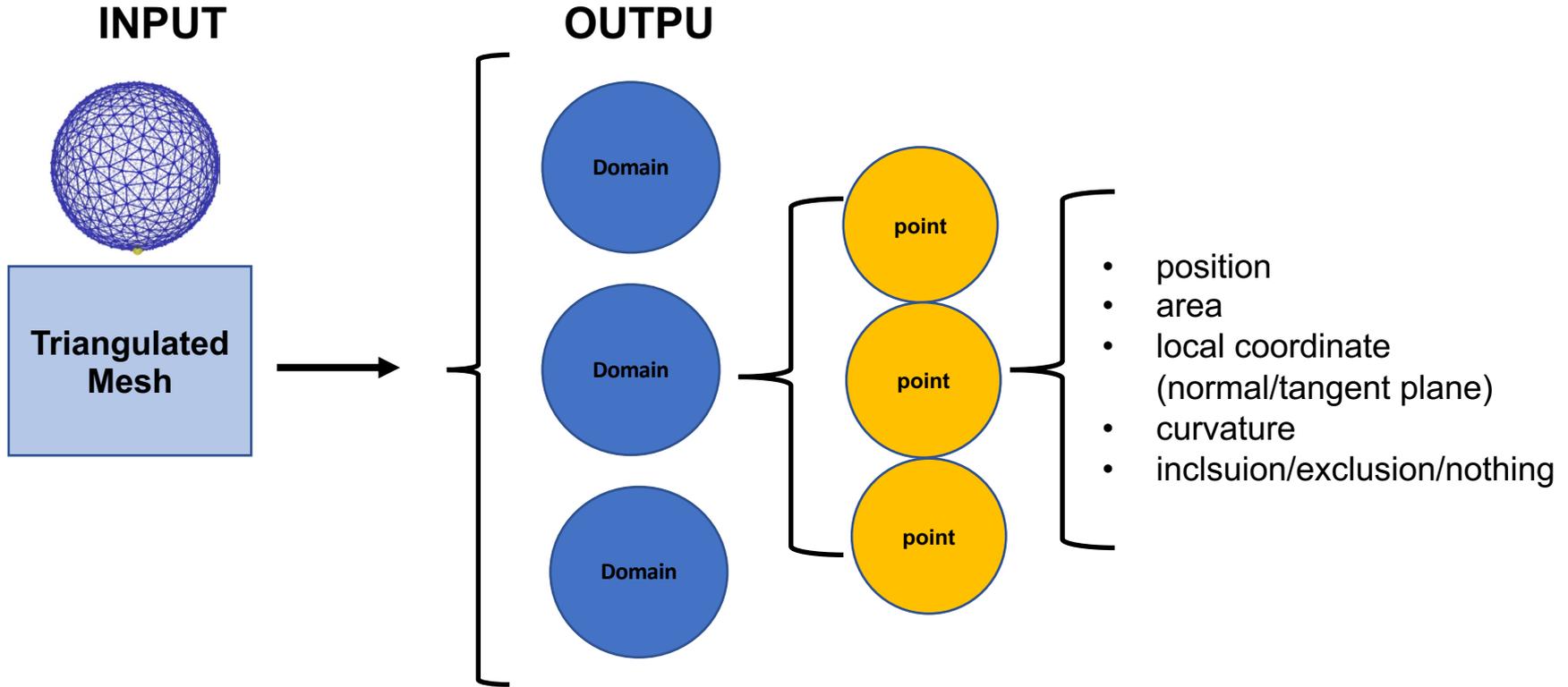
Coordinate file of the full system.



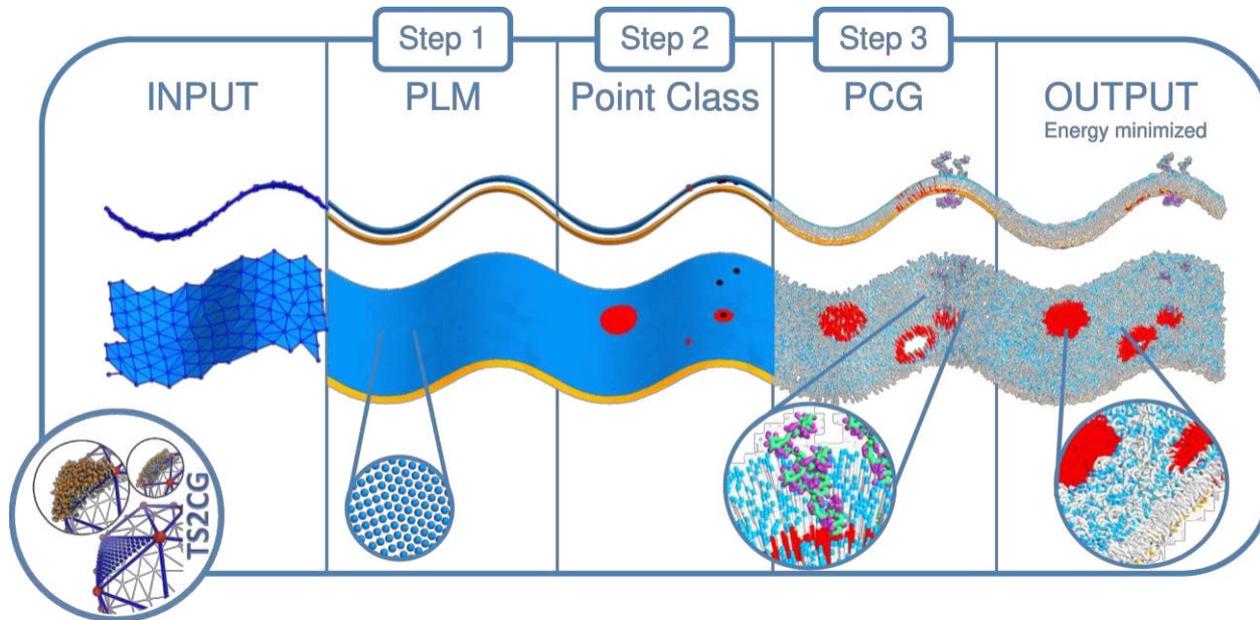
# Membrane shape and lateral organization are coupled



# Pointillism: PLM



# TS2CG v2.x



Pezeshkian, et al, Nat. Commun **11**, 2296 (2020).

Fabian Schuhmann, et al, JCTC (2025) doi: <https://doi.org/10.1101/2025.04.16.649160>

<https://github.com/weria-pezeskian/TS2CG-v2.0>;

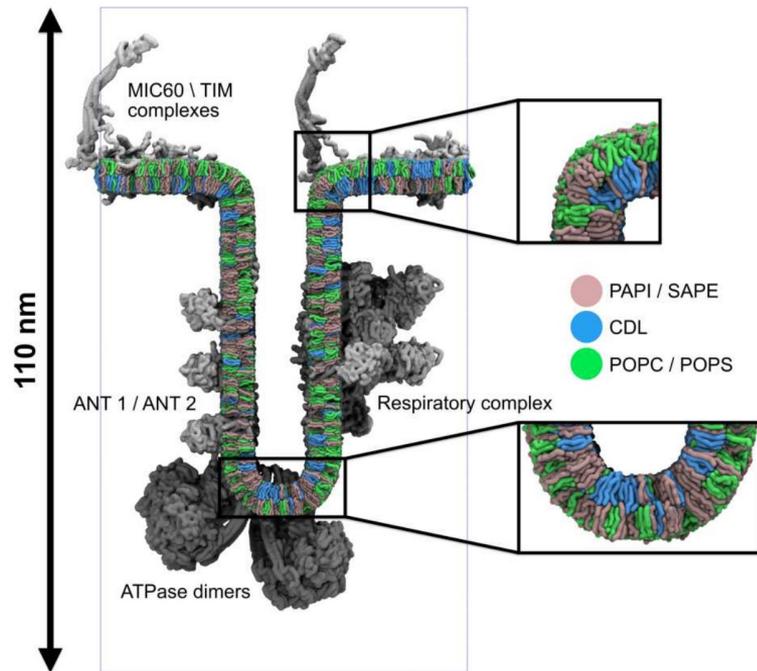
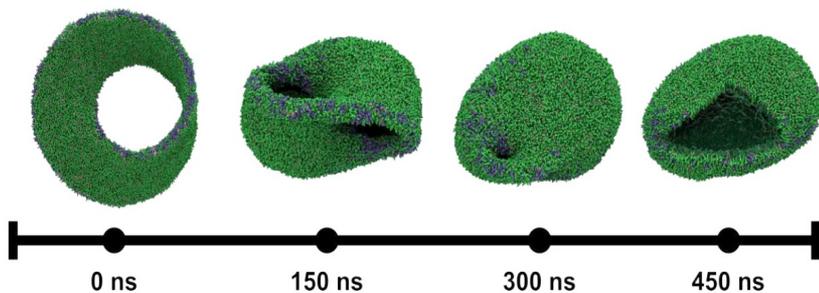
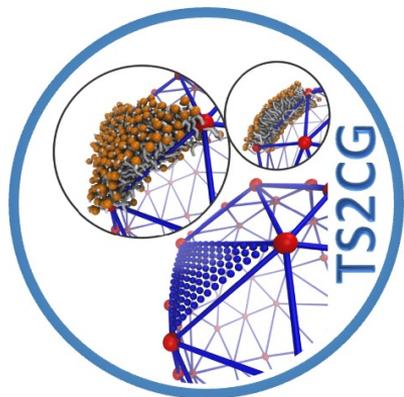
# TS2CG 2.0 Adds “The Point Class API”

TS2CG 2.0 is distributed through PyPI, so install via pip.

DAI (**D**omains **A**round **I**nclusions): circular lipid domains around proteins or around any arbitrary point (DAI).

DOP (**D**istribution-based **O**ptimized **P**lacement): assigning lipids based on curvature preference.

INU (**I**nclusion **U**dater): inserting membrane proteins based on curvature preference.



Pezeshkian, et al, Nat. Commun **11**, 2296 (2020).

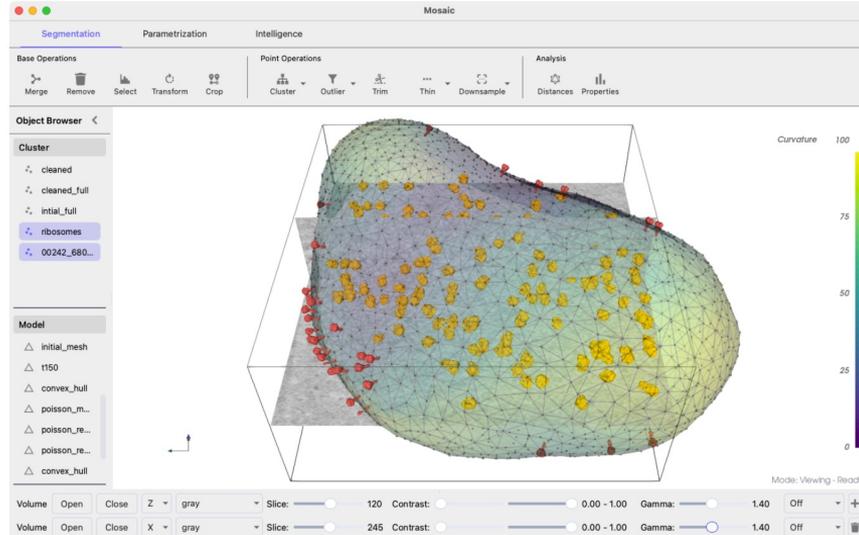
Fabian Schuhmann, et al, (2025) doi: <https://doi.org/10.1101/2025.04.16.649160>

<https://github.com/weria-pezeskian/TS2CG-v2.0>;

# If you are dealing with cryo-ET data



**mosaic**

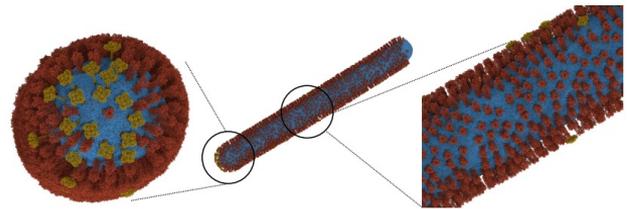
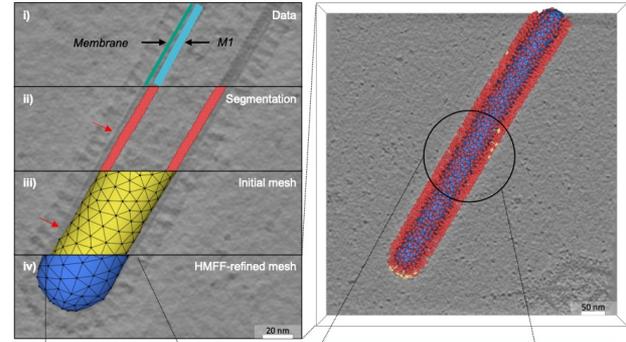
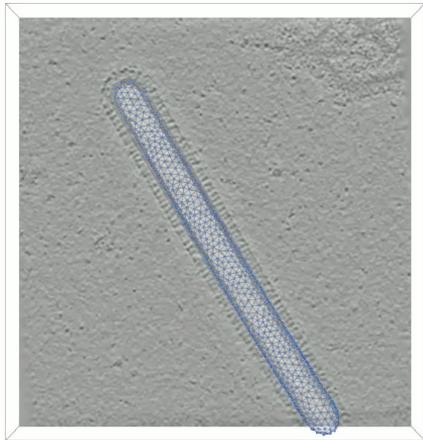


V, Maurer, et al, (2025) doi: <https://doi.org/10.1101/2025.05.24.655915>

Helfrich Monte Carlo Flexible Fitting: physics-based, data-driven cell-scale simulations;

# Influenza A virus particles

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V, Maurer, et al, (2025) doi: <https://doi.org/10.1101/2025.05.24.655915>  
Helfrich Monte Carlo Flexible Fitting: physics-based, data-driven cell-scale simulations;

**Any ideas for future development?**

---

# Acknowledgments

---

Siewert J Marrink  
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Melanie König  
Tsjerk A. Wassenaar  
Neda Rahmani  
Isabell Lindahl  
Chelsea M Brown  
Christopher Brasnett  
Dimitrios Anastasiou  
Adrià Bravo Vidal  
Beatrice Geiger  
Paulo Cesar Telles de Souza  
Fabian Grünewald

## My Group Members

Neda Rahmani  
Fabian Schuhmann  
Adrià Bravo Vidal  
Beatrice Geiger  
Isabell Lindahl  
Brian Ratnasinghe



<http://commicgroup.ku.dk>



@Wpezeshkian



novo  
nordisk  
fonden

```

include protein.gro
[Lipids List]
;LipidName  RatioUp  RatioDown  Area/Lipid
Domain 0
POPC        0.5      0.5        0.63
POPE        0.5      0.5        0.64
End
Domain 1
POPC        0.5      0.5        0.63
POPE        0.5      0.5        0.64
End
[Shape Data]
ShapeType   Flat
Box         40    40    40
Density     2     2
Thickness   3.8
WallRange   0     1     0     1
End
[Protein List]
;ProteinName  Incl.Id  Surface_Coverage  0  0  z-position
STxB          1        0.5                0  0  -1.1
end Protein

```

Description Martini Map CG

Version Martini 3

;Martini 3 lipid library for TS2CG 2.0

;Made by Reinier de Vries on 31-03-2021. Last updated: 04-05-2021

;NOTE: Bead atom names don't match current Martini 3 bead atom names, use `-maxwarn` in GROMACS

[DAPC]

```
1 NC3 0 0 1
2 P04 0 0 0
3 GL1 0 0 -1
4 GL2 0 0.5 -1
5 D1A 0 0 -2
6 D2A 0 0 -3
7 D3A 0 0 -4
8 D4A 0 0 -5
9 C5A 0 0 -6
10 D1B 1 0 -2
11 D2B 1 0 -3
12 D3B 1 0 -4
13 D4B 1 0 -5
14 C5B 1 0 -6
```

[POPC]

```
1 NC3 0 0 1
2 P04 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 0 -4
8 C4A 0 0 -5
9 C1B 1 0 -2
10 C2B 1 0 -3
11 C3B 1 0 -4
12 C4B 1 0 -5
```

# Useful links

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**Source code:** <https://github.com/weria-pezeskian/TS2CG-v2.0>

**Tutorials:** <https://github.com/weria-pezeskian/TS2CG-v2.0/wiki/Tutorial>

PointClass Documentation:

[https://weria-pezeskian.github.io/TS2CG\\_python\\_documentation/](https://weria-pezeskian.github.io/TS2CG_python_documentation/)

# Tutorials and the manual

The screenshot shows a GitHub Wiki page for 'Workshop 2024'. The page title is 'Workshop 2024' and it was last edited by Weria Pezeshkian on Dec 6, 2024, with 76 revisions. The main heading is 'Advances in Molecular Modelling Workshop 2024'. The introductory text welcomes users to the FreeDTS Tutorial section and outlines the progression from basic examples to more complex scenarios. A 'List of the tutorials' section lists four tutorials: Vesicle, Framed membrane, Proteins, and Custom simulation. A 'Required Software' section mentions ParaView, VMD, and a C++ compiler supporting OpenMP. On the right side, there is a 'Wiki Navigation' sidebar with links to Home, Documentation (User Manual: version 2 and version 1), and Tutorials (Workshop 2024 with version 2, Tutorials with version 1, and Tutorials with version 2 (2025)). There is also a 'Clone this wiki locally' button with a URL: https://github.com/weria-pezeskian/FreeDTS/wiki/Workshop-2024.

github.com/weria-pezeskian/FreeDTS/wiki/Workshop-2024

## Workshop 2024

Weria Pezeshkian edited this page on Dec 6, 2024 · [76 revisions](#)

### Advances in Molecular Modelling Workshop 2024

Welcome to the FreeDTS Tutorial section of the Advances in Molecular Modeling Workshop 2024! This guide is here to introduce you to FreeDTS Version 2 and show you how to simulate membranes at the mesoscale. In a series of tutorials, you'll progressively learn to set up, run, and analyze FreeDTS simulations, beginning with basic examples and advancing to more complex scenarios. The final tutorial even covers modifying the FreeDTS source code for custom simulation needs.

#### List of the tutorials

If you're new to dynamically triangulated surfaces, especially with FreeDTS, start with the tutorials at the top and work your way down. However, if you're already familiar with the basics and have some coding experience, you may want to begin with the [fourth tutorial](#) or doing the first and jumping to the fourth.

- Tutorial I: [Vesicle](#)
- Tutorial II: [Framed membrane](#)
- Tutorial III: [Proteins](#)
- Tutorial IV: [Custom simulation](#)

#### Required Software

For visualisation: preferably [ParaView](#), or [VMD](#) and C++ compiler supporting [OpenMP](#).

Pages 7

#### Wiki Navigation

- Home
- Documentation
  - [User Manual: version 2](#)
  - [User Manual: version 1](#)
- Tutorials
  - [Workshop 2024 with version 2](#)
  - [Tutorials with version 1](#)
  - [Tutorials with version 2 \(2025\)](#)

Clone this wiki locally

<https://github.com/weria-pezeskian/FreeDTS/wiki/Workshop-2024>

If you are interested, you can follow tutorials to learn how to perform simulations using FreeDTS and conduct research on biomembranes.

<https://github.com/weria-pezeskian/FreeDTS/wiki/Workshop-2024>