

# Visualizing and exploring complex molecular simulations

Computer graphics in the service of biochemists

Maxime MARIA

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March 20, 2024

# Who am I?

Maxime MARIA, 33 years old

maxime.marie@unilim.fr

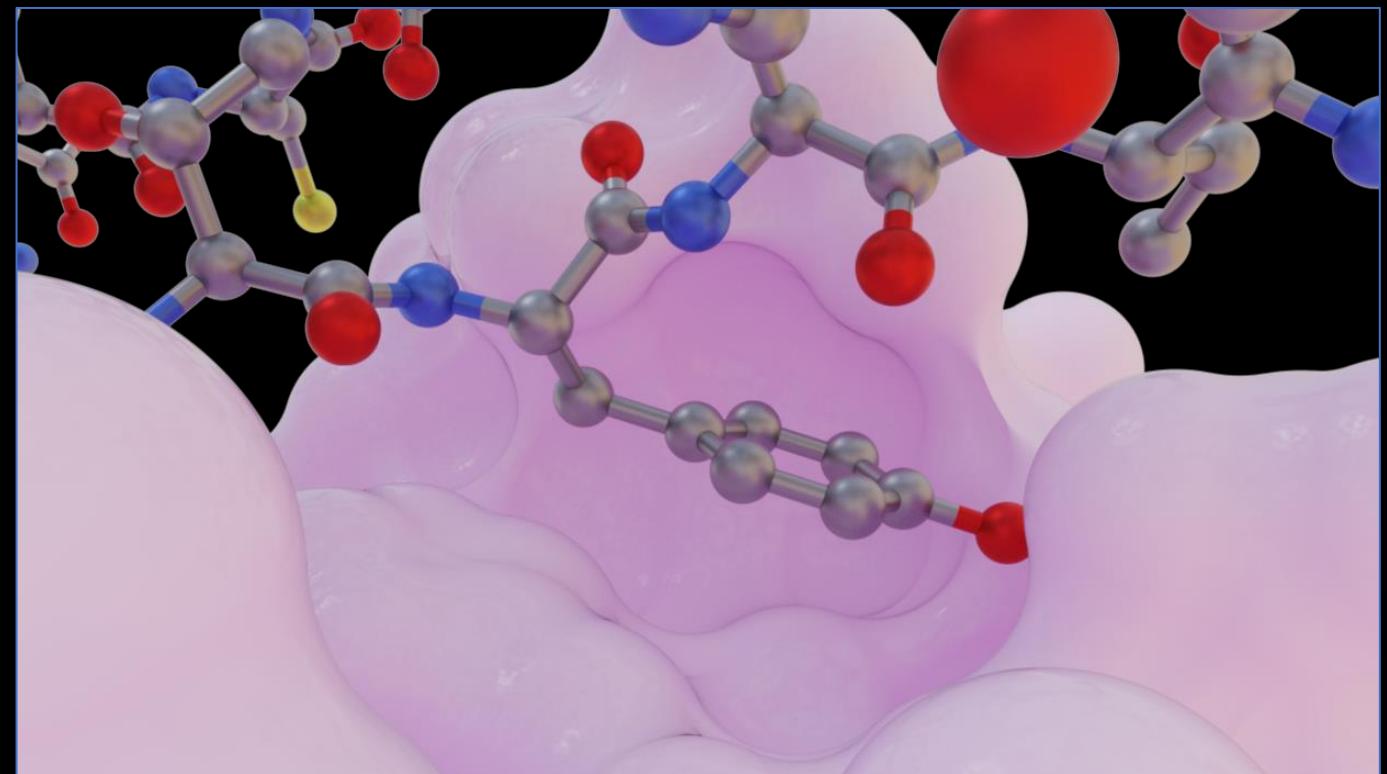
- Associate professor (Maître de conférences) – XLIM/ASALI/SIR, University of Limoges
- Associated researcher – GBCM Lab (Genomics, Bioinformatics, Molecular Chemistry), CNAM Paris

Specialty: Computer Graphics

- Image synthesis (rendering)
- High-performance computing
- Geometric data structures

Application: molecular visualization

- Realtime 3D exploration
- High-quality illustration
- Structure analysis



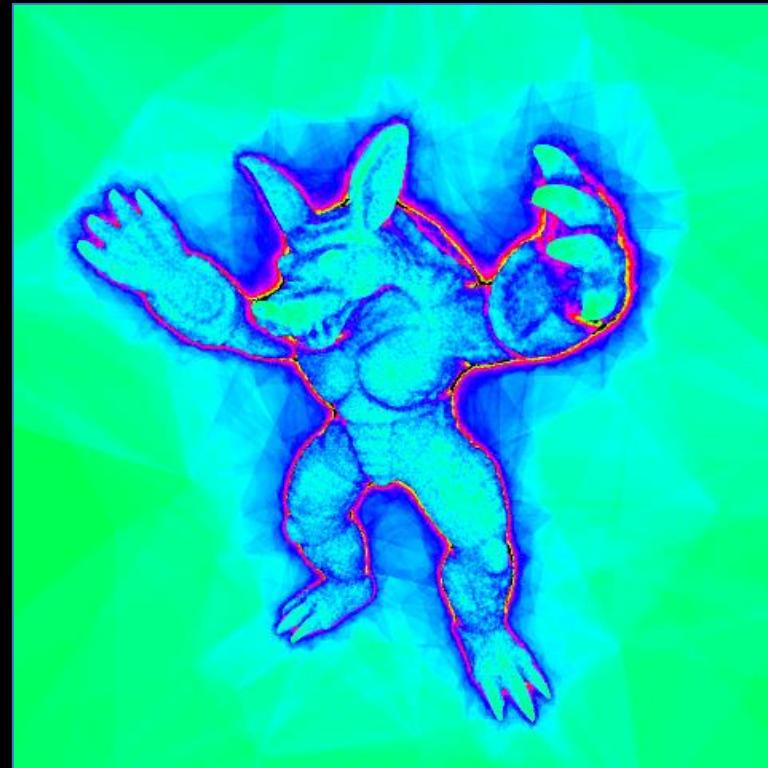
2016: XLIM, University of Poitiers

## New type of acceleration structure for ray-tracing

- Constrained Convex Space Partition (CCSP): kind of graph made up of convex volumes



*CCSP for architectural environments*

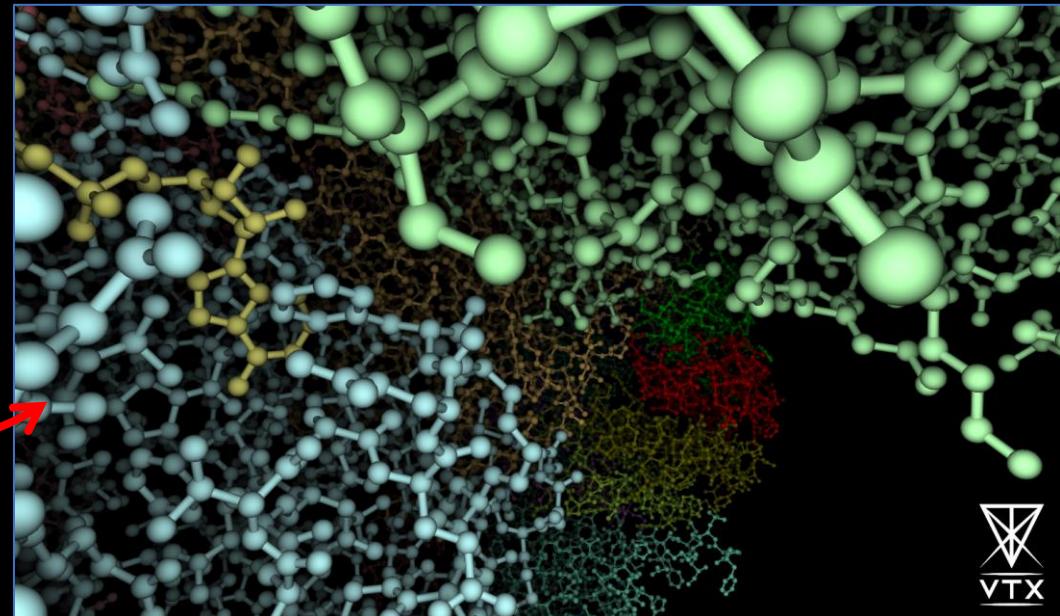
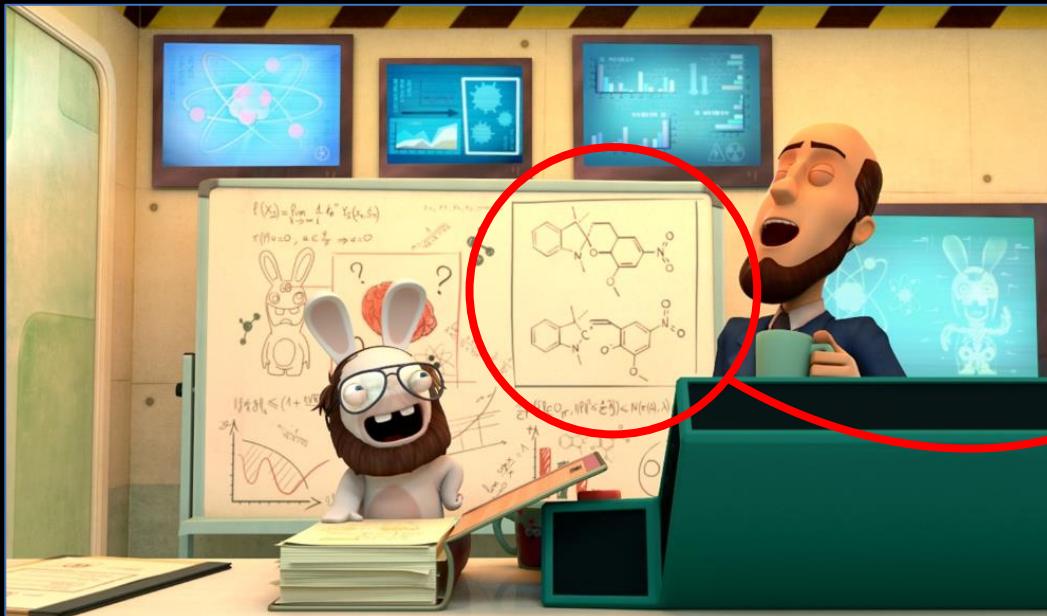


*Constrained Delaunay Tetrahedralization*

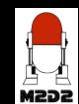
# PostDoc (2/2)

2019: GBCM Lab (Genomics, Bioinformatics, Molecular Chemistry), CNAM Paris  
LCT (Laboratory of Theoretical Chemistry), Sorbonne University, Paris

Computer Graphics for Bio/Chemo-informatics



Resignation because I had a tenured faculty position, but we are still working together!



le cnam

LCT  
Laboratoire de Chimie Théorique

S SORBONNE  
UNIVERSITÉS

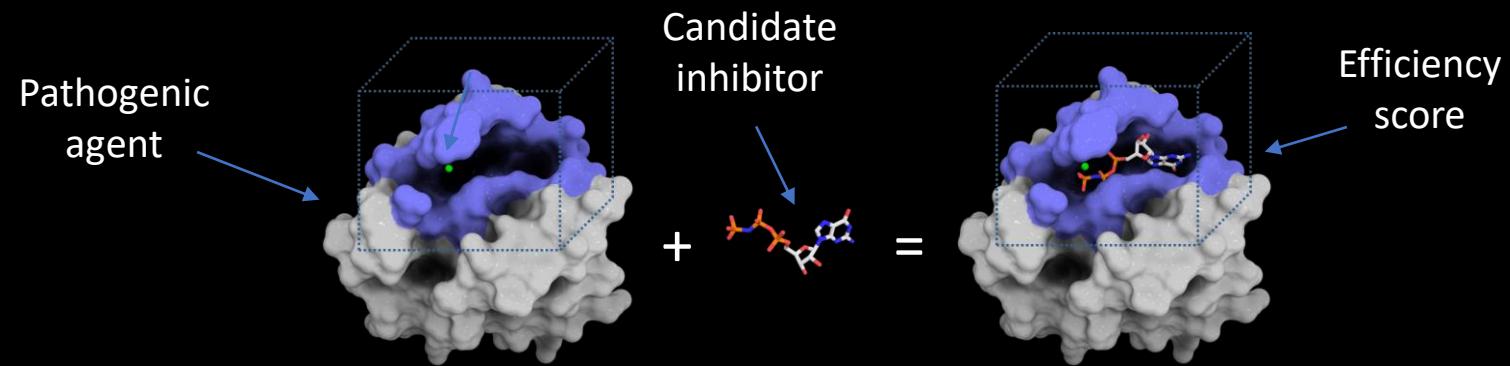
# Why molecular visualization?

# Molecular visualization

Nowadays, visual analysis of molecular simulations is essential in drug-design

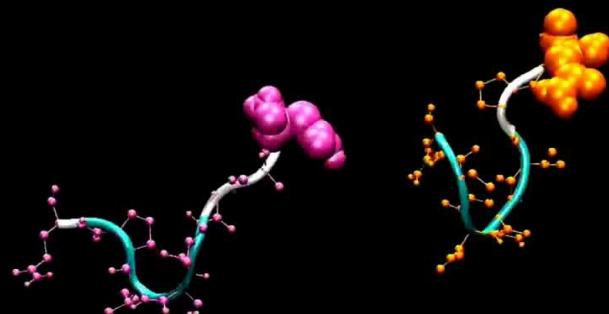
Docking: to search for candidate inhibitors of pathogens

- Reduces the number of *in vivo* tests required



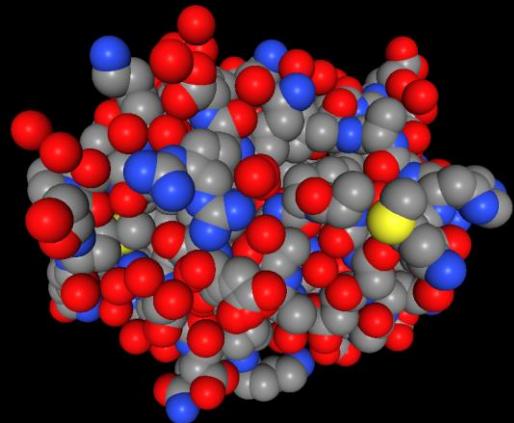
Molecular dynamics: to understand molecules behavior

- And to analyze their interactions

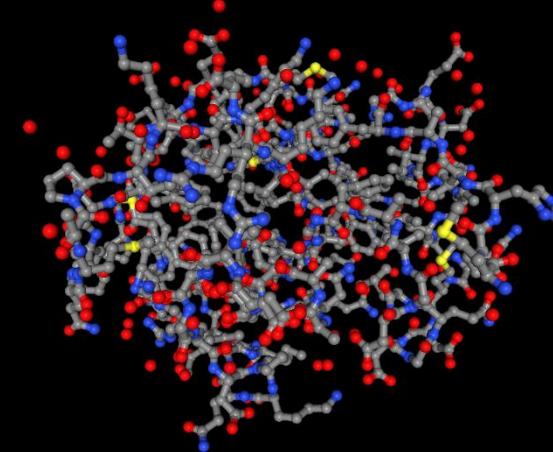


# Different representations

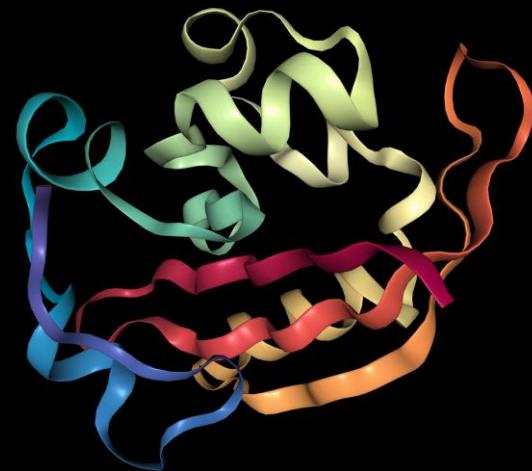
Depending on what the user wants to study



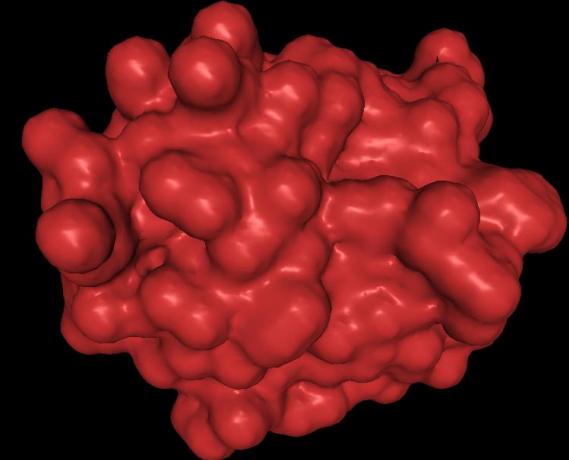
van der Walls (vdW)



Ball and Stick



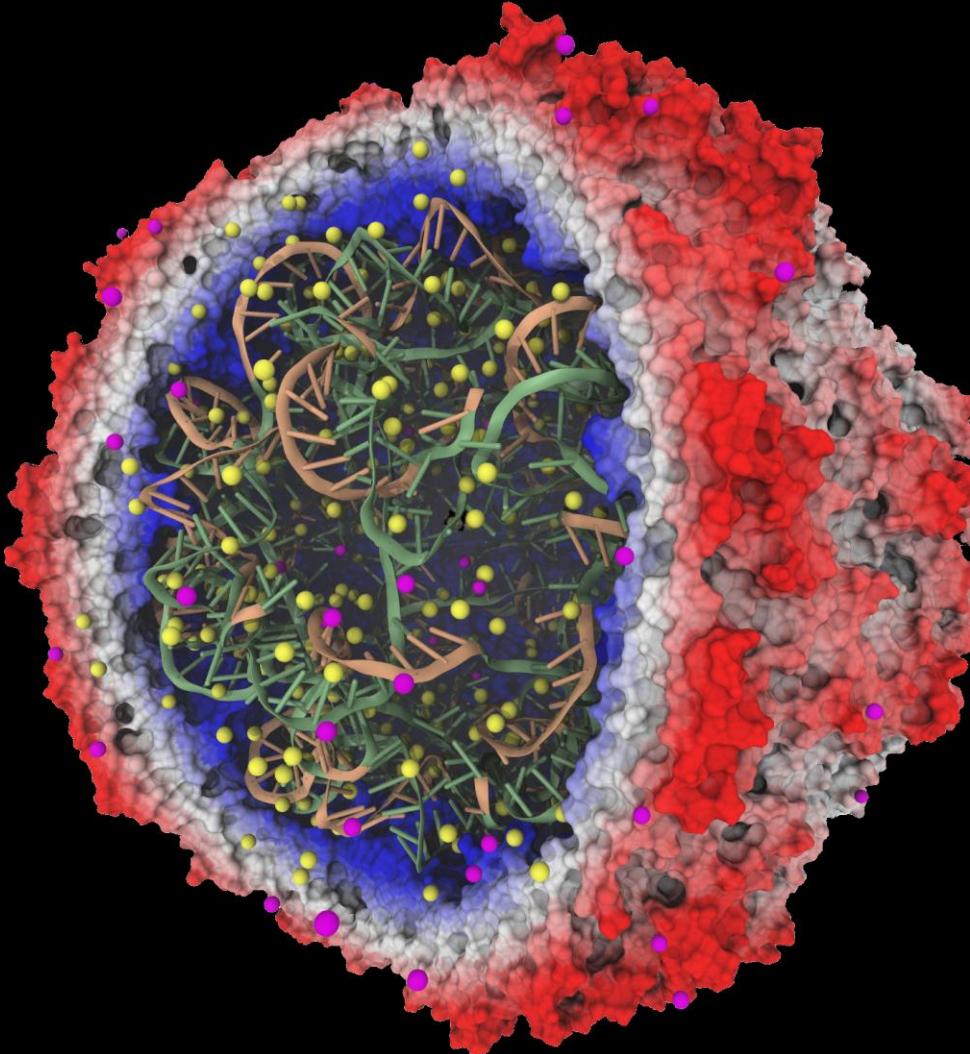
Cartoon



Surfaces



# Different representations

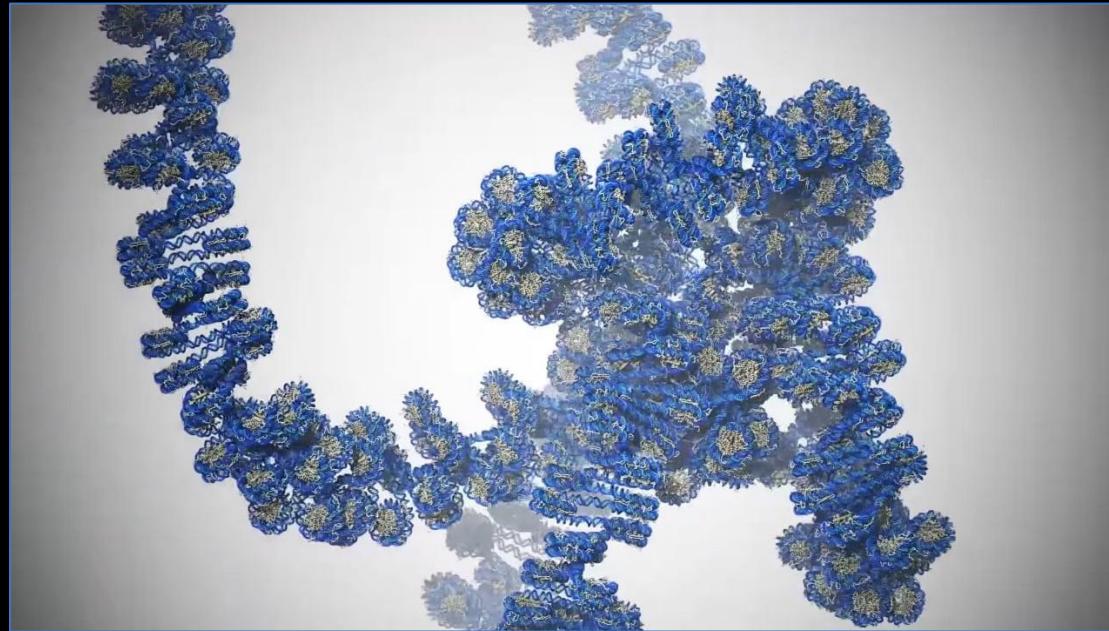


# Increasingly complex simulations

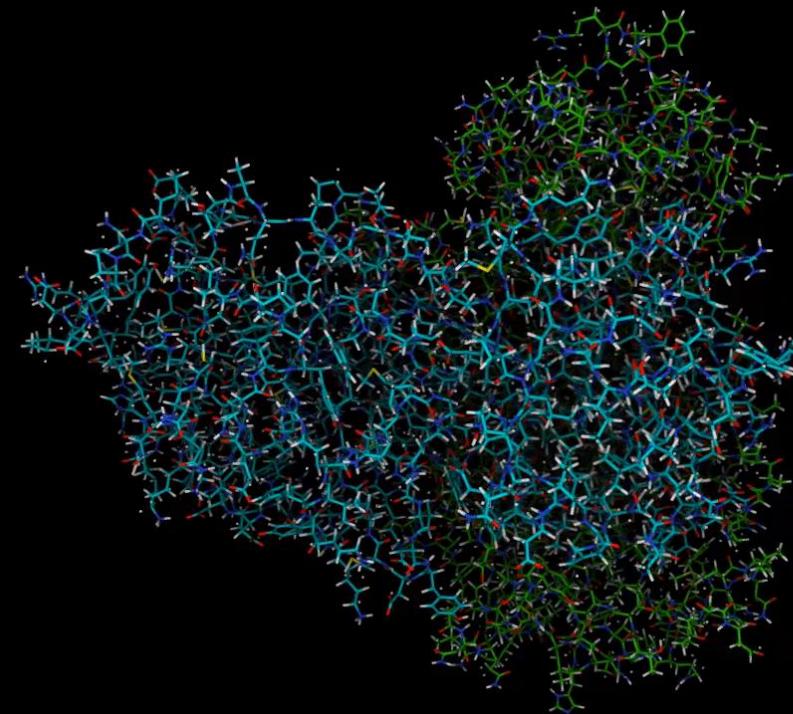
Systems composed of millions of atoms (even billions)

Molecular dynamics (simulation rate of  $10^{-15}$ s)

- Each atom moves with each step
- Need to display and manipulate interactively



Simulation of a single human gene > 1 billion of atoms  
©Los Alamos National Laboratory



A molecular dynamics  
(displayed at 30 steps/second)



# What do we do in Limoges?

# What do we do in Limoges?

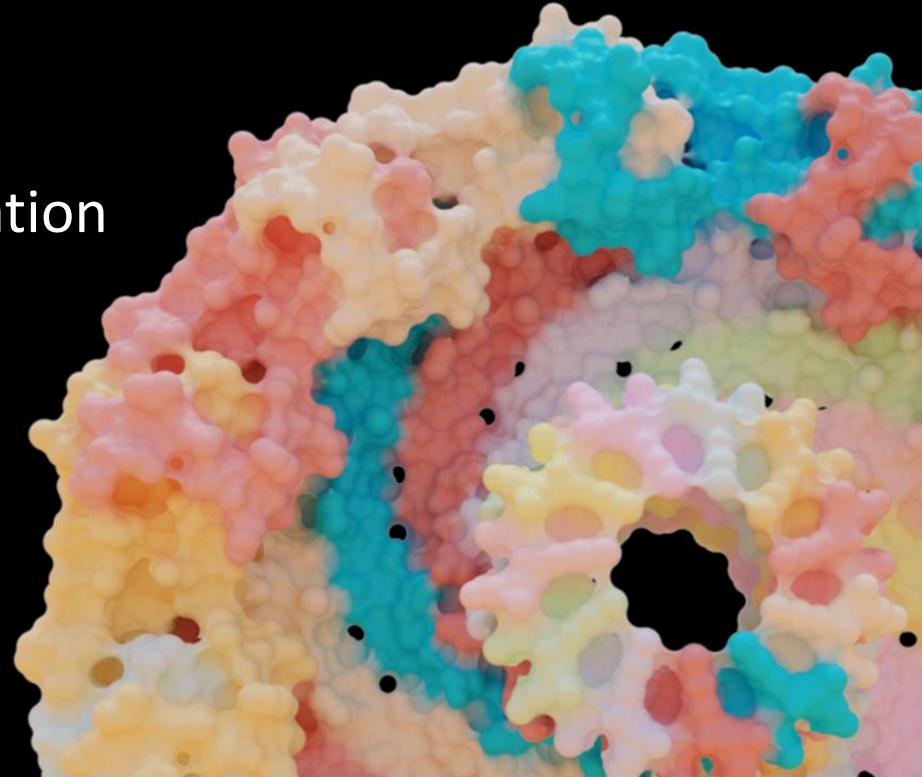
VTX: high-performance molecular visualization software

Efficient construction of Solvent Excluded Surface (SES)

Apollonius diagrams computation

Computer-aided generation of molecular simulation illustration

UDock2: Protein-protein docking





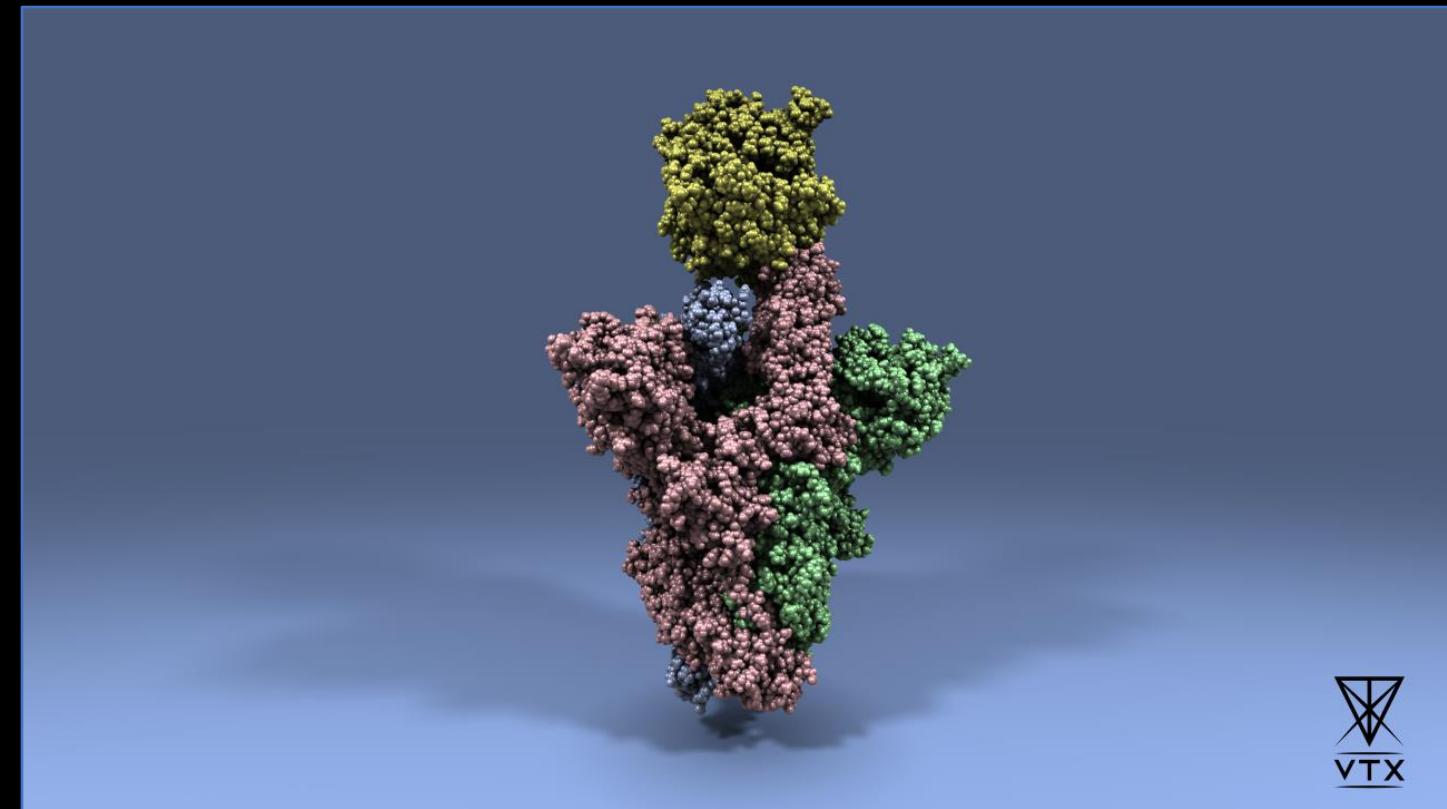
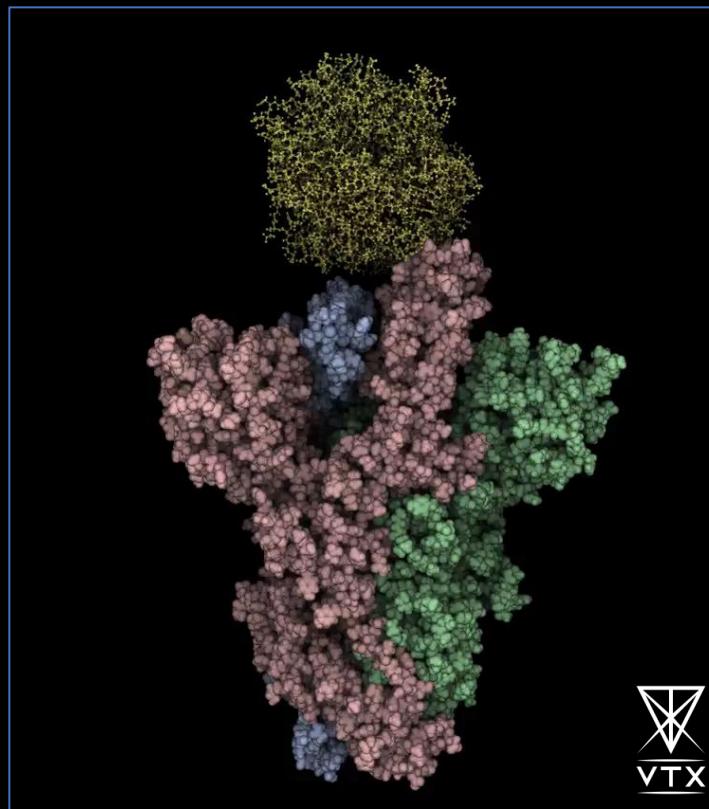
**VTX: high-performance molecular visualization software**

# VTX: a new software to visualize molecular systems

Realtime visualization/exploration + High-quality rendering for illustration

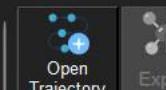
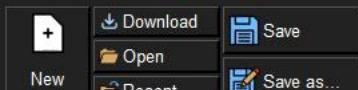
Complex molecular systems (millions of atoms ++)

Open-source (for academics ☺)

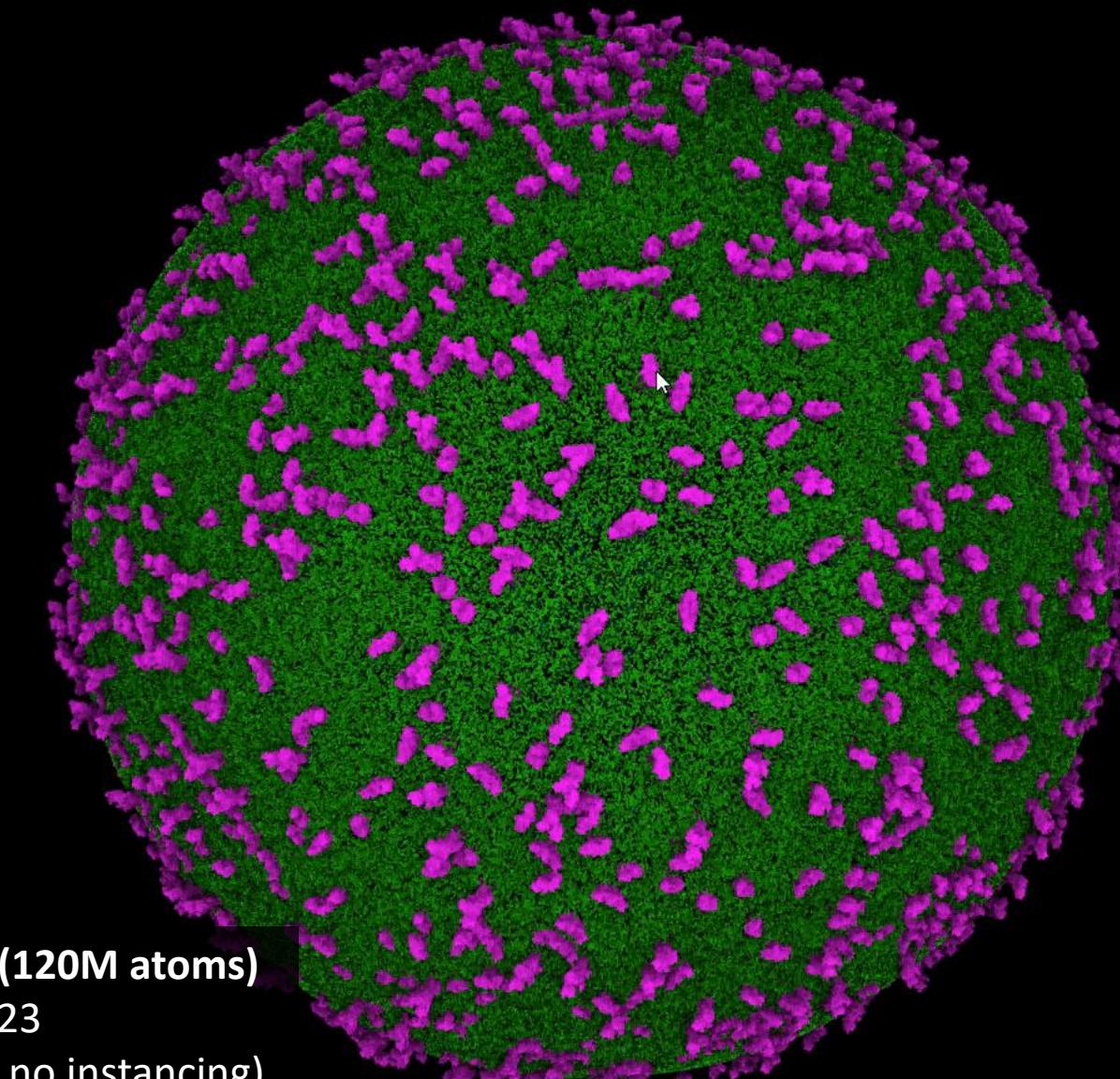
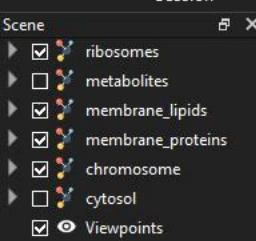


Interaction ACE-2/Spike (SARS-CoV-2)

File Edit Visualization Tools



[https://x.com/VTX\\_mol/status/1669421000109314050?s=20](https://x.com/VTX_mol/status/1669421000109314050?s=20)



**Navigation in mycoplasma whole cell (120M atoms)**

GGMM workshop, may 2023

Real-time capture (Nvidia RTX 2080M, no instancing)

Data: ©Marrink S. J. ©CG Martini



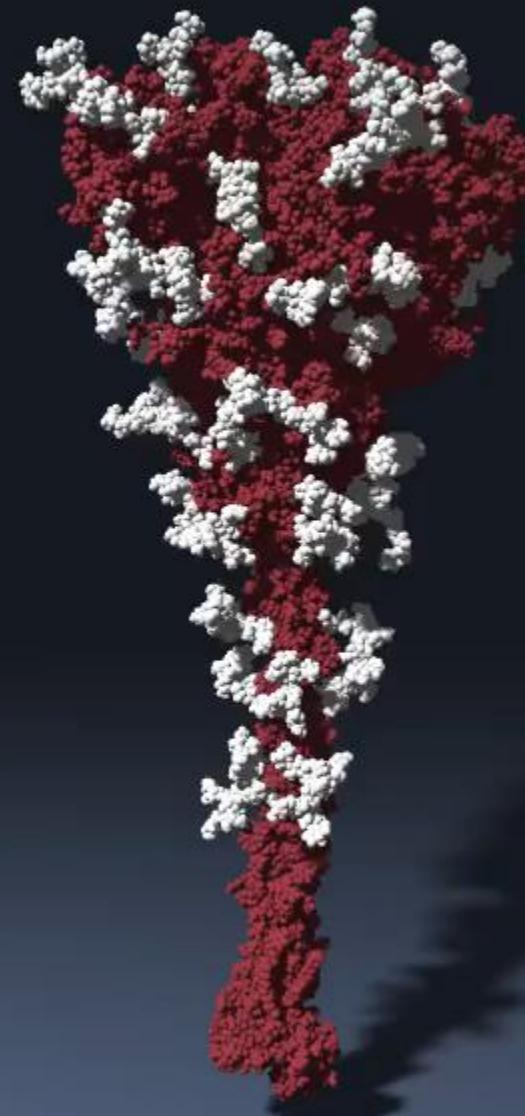
Status bar

# SARS-CoV-2 Spike/membrane connection

TV Documentary for Arte, may 2020

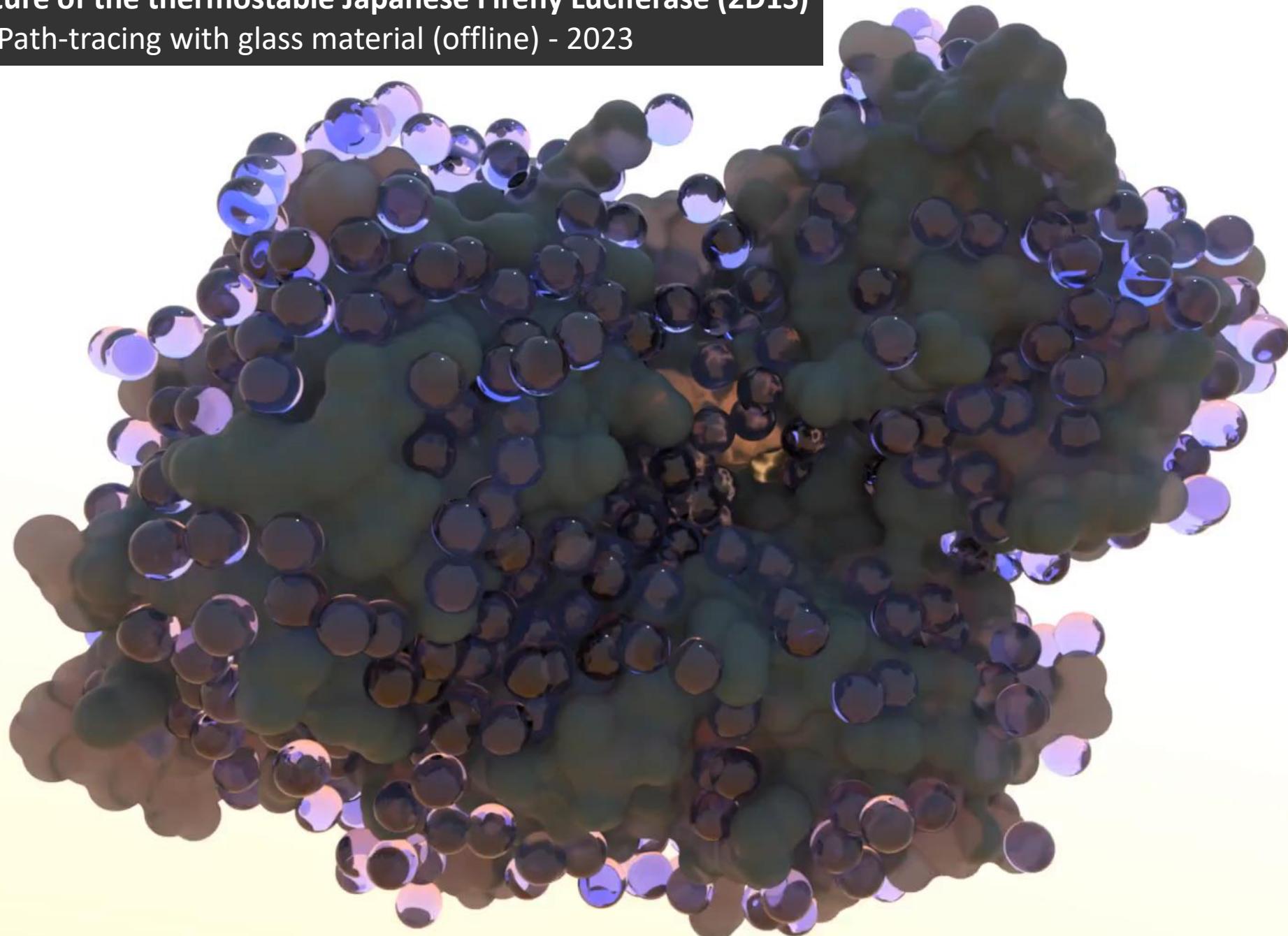
Offline rendering

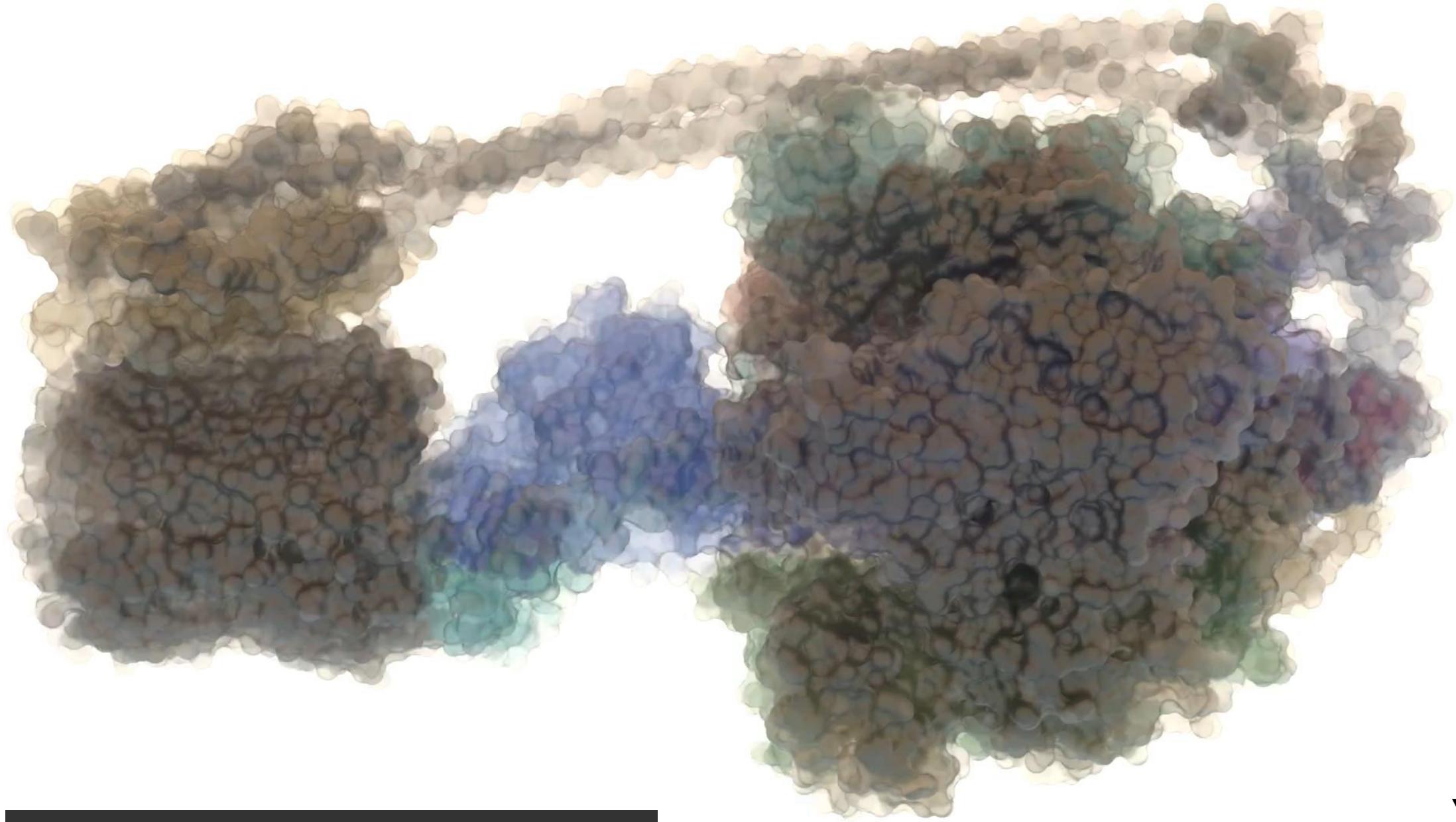
Data: ©AmaroLab ©LCT



# Crystal structure of the thermostable Japanese Firefly Luciferase (2D1S)

Path-tracing with glass material (offline) - 2023





I don't remember but I love it 😊

Path-tracing molecular dynamics (offline) - 2023



# What do we do in Limoges?

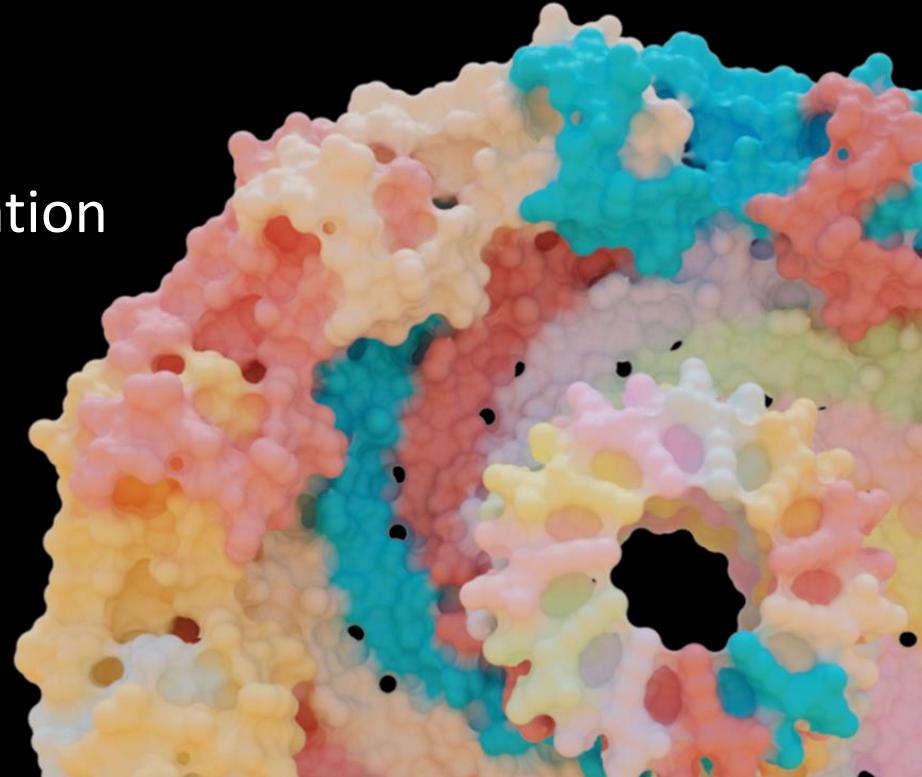
VTX: high-performance molecular visualization software

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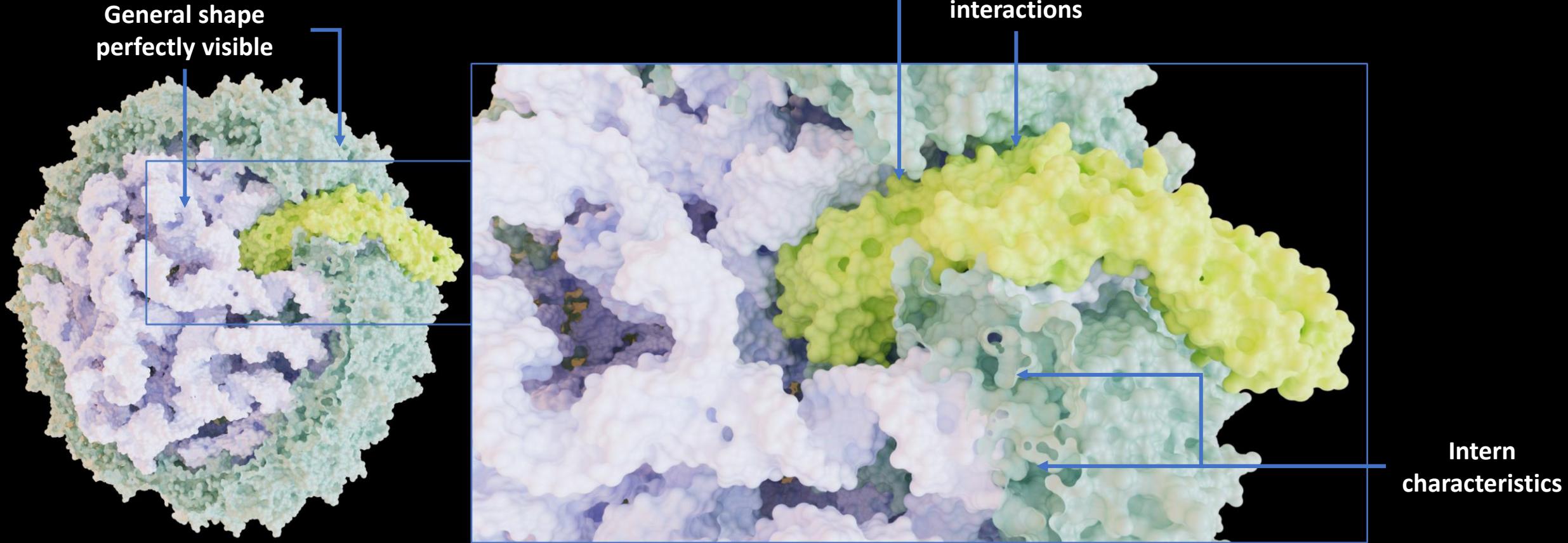
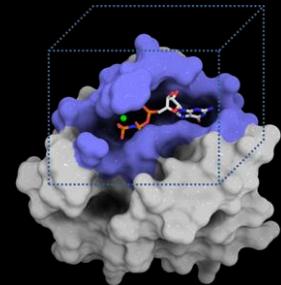
UDock2: Protein-protein docking



# Solvent Accessible/Excluded Surface (SAS/SES)

Useful representations (*e.g.* for docking):

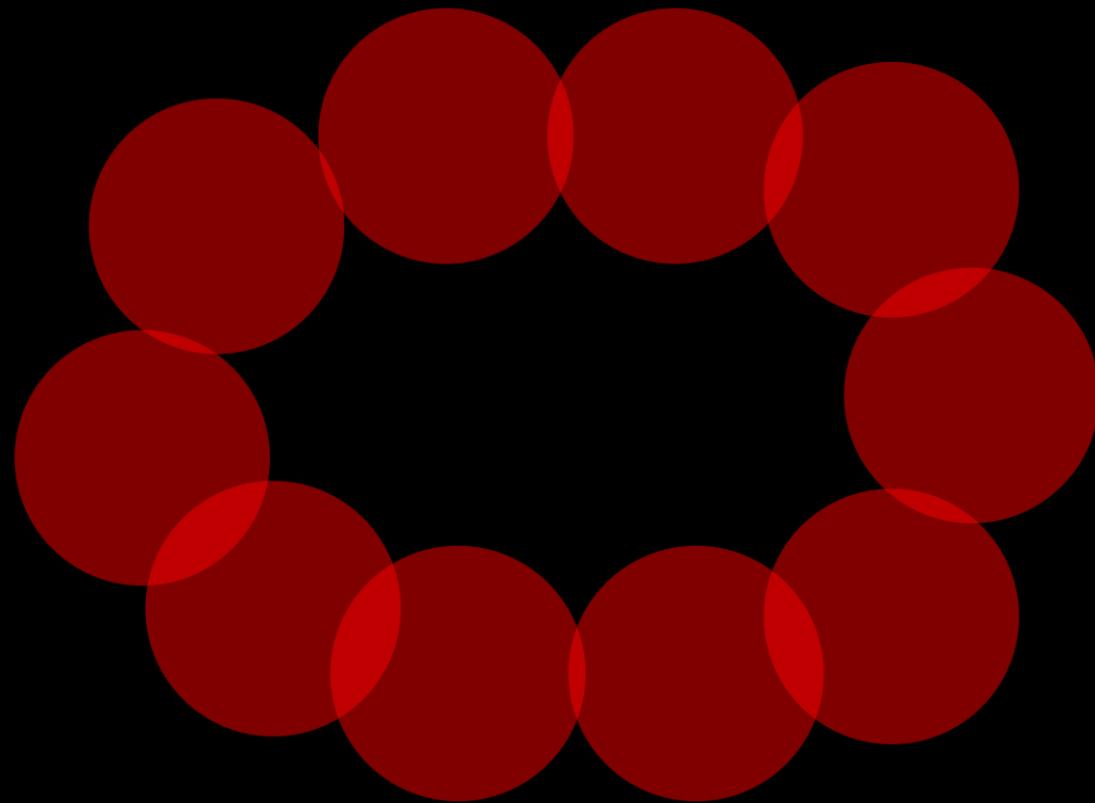
- Delimit the space in which a solvent can enter



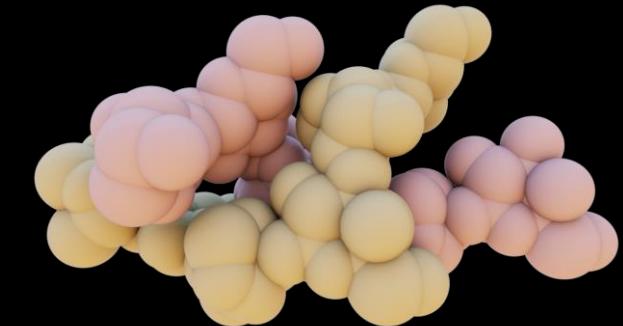
# Solvent Accessible/Excluded Surface (SAS/SES)

Surfaces traced by a probe rolling on the van der Walls atoms

●  $vdW$



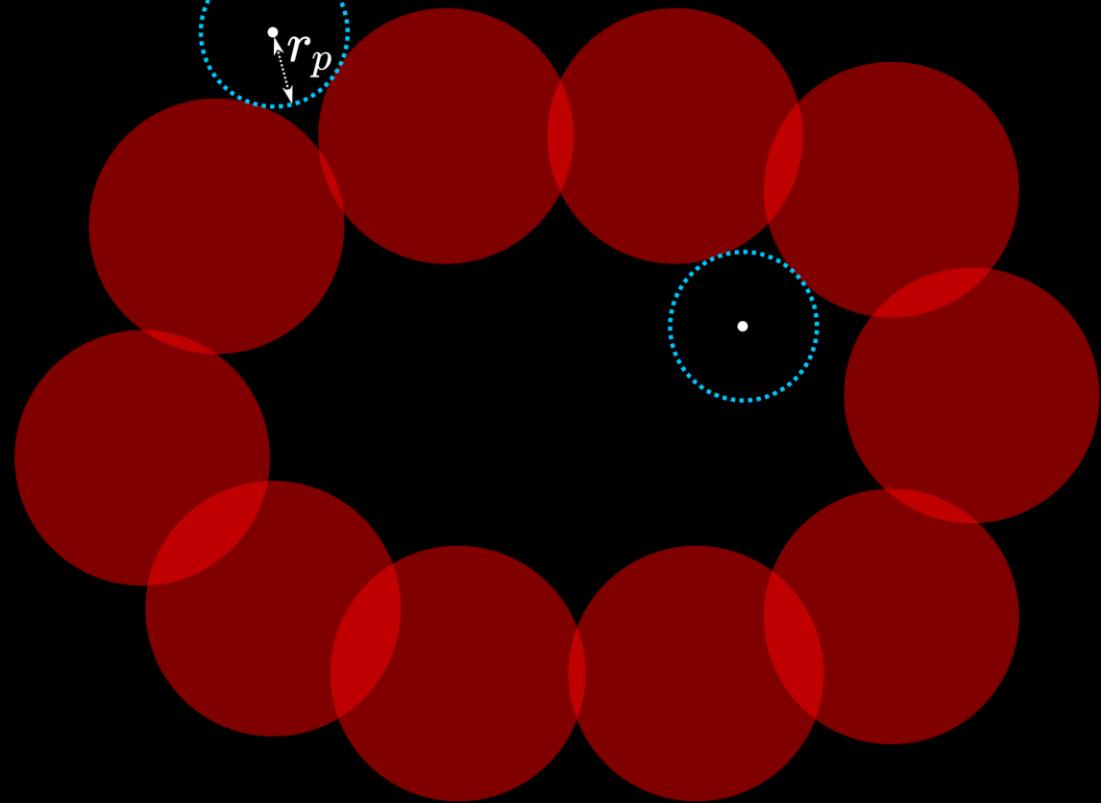
$vdW$



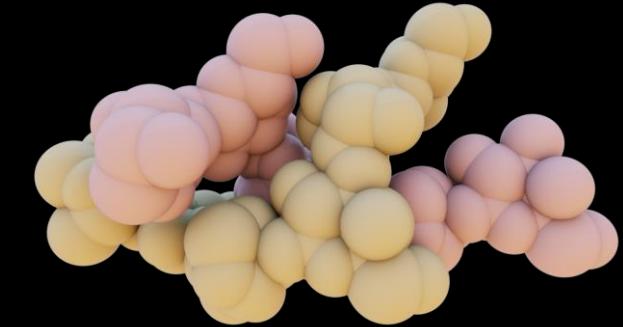
# Solvent Accessible/Excluded Surface (SAS/SES)

Surfaces traced by a probe rolling on the van der Walls atoms

 Rolling probe  
 vdW



vdW



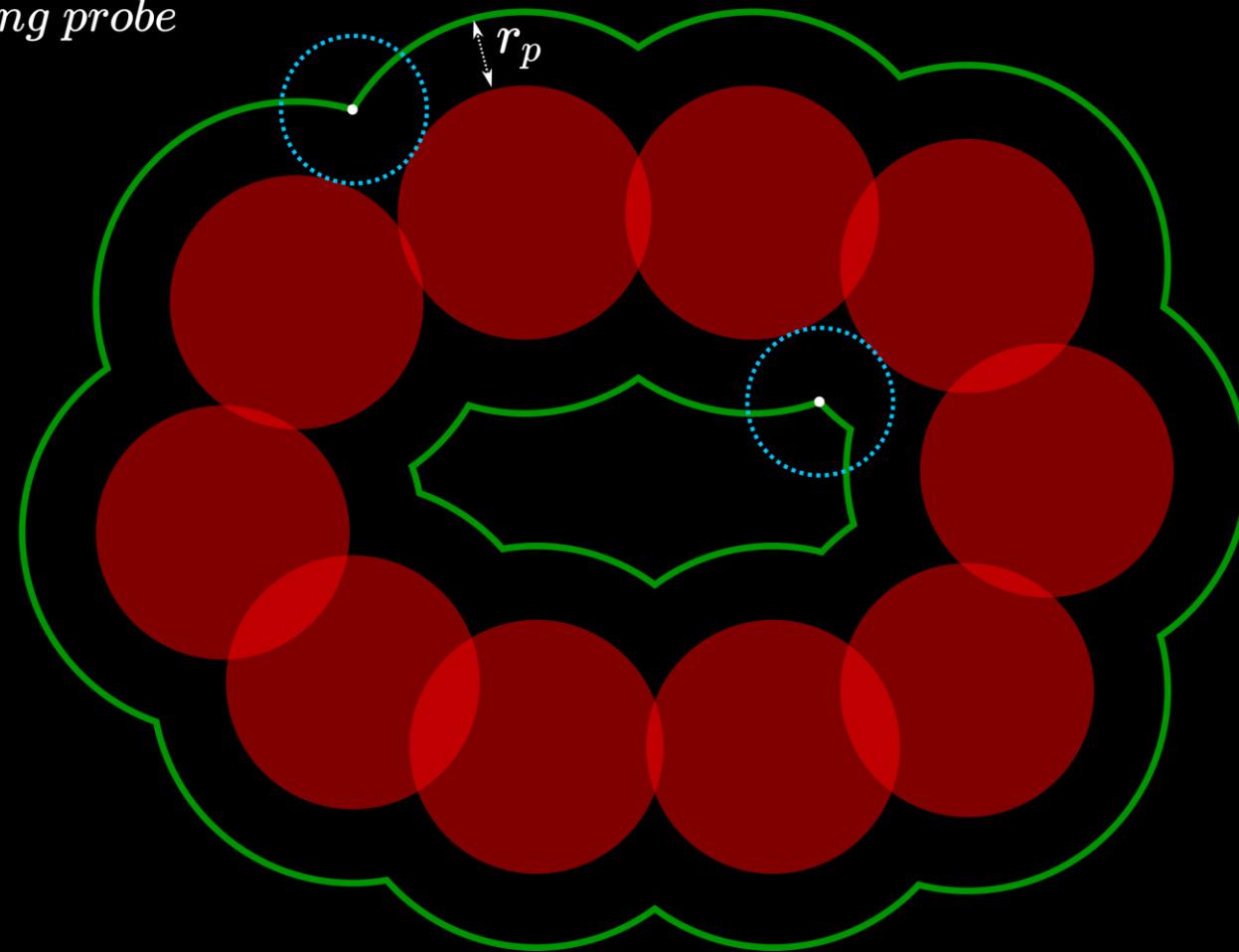
# Solvent Accessible/Excluded Surface (SAS/SES)

Surfaces traced by a probe rolling on the van der Walls atoms

 Rolling probe

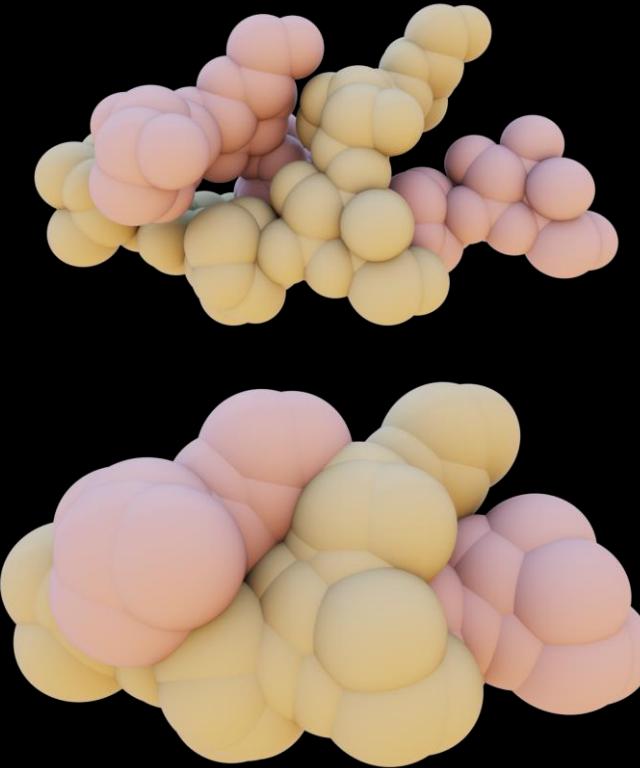
 vdW

 SAS



vdW

SAS



# Solvent Accessible/Excluded Surface (SAS/SES)

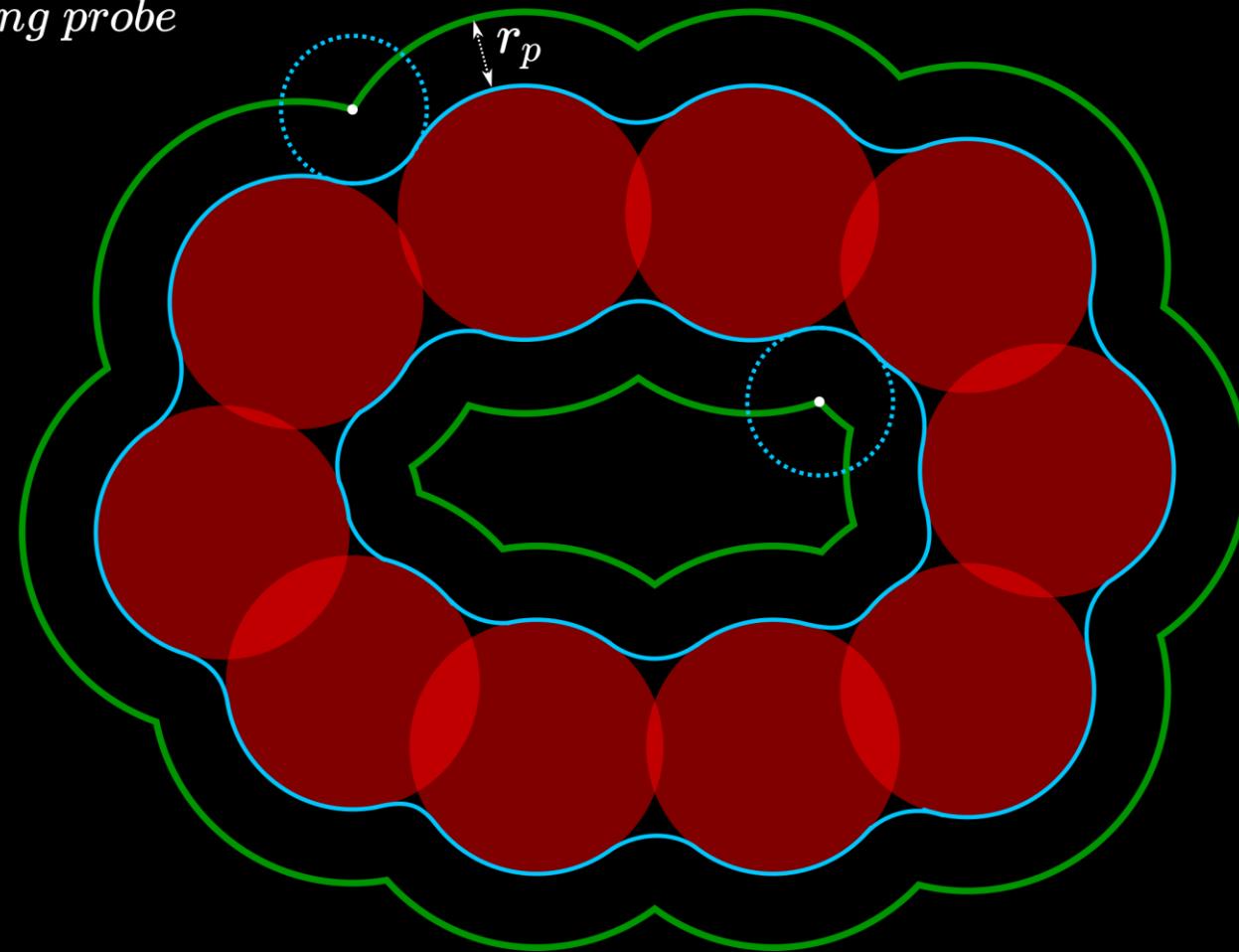
Surfaces traced by a probe rolling on the van der Walls atoms

 Rolling probe

 vdW

 SAS

 SES



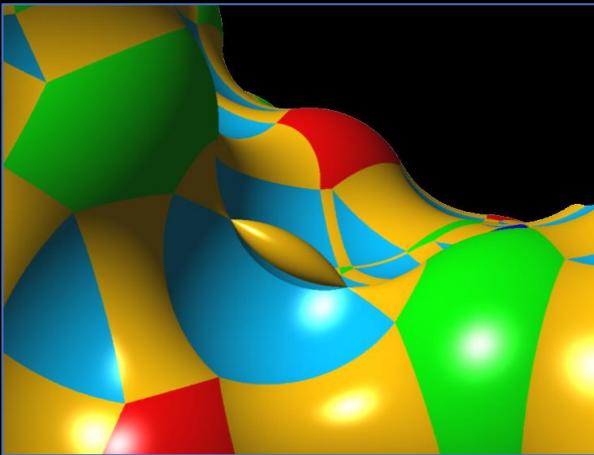
*vdW*

*SAS*

*SES*

# Geometric singularities

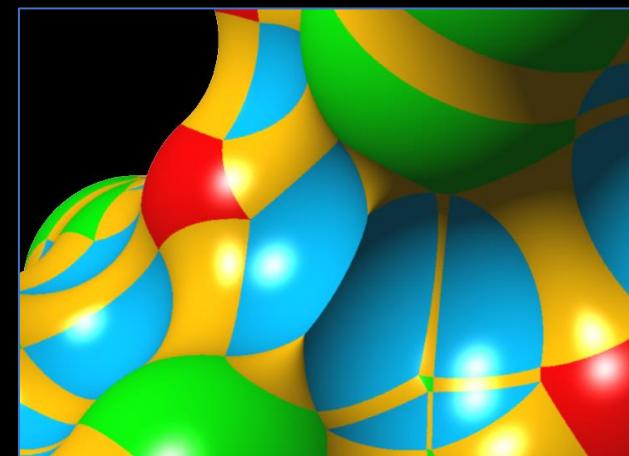
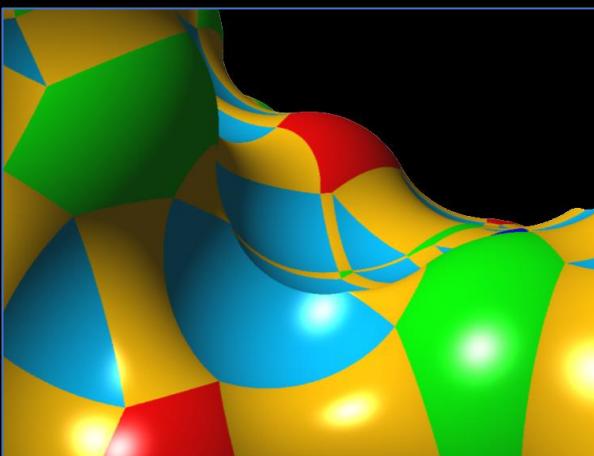
Self-intersecting (T)



Intersection of two (TS)



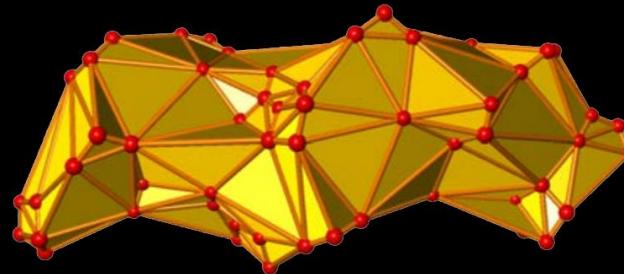
Usually handled in a post-process



# SES construction: analytic approaches

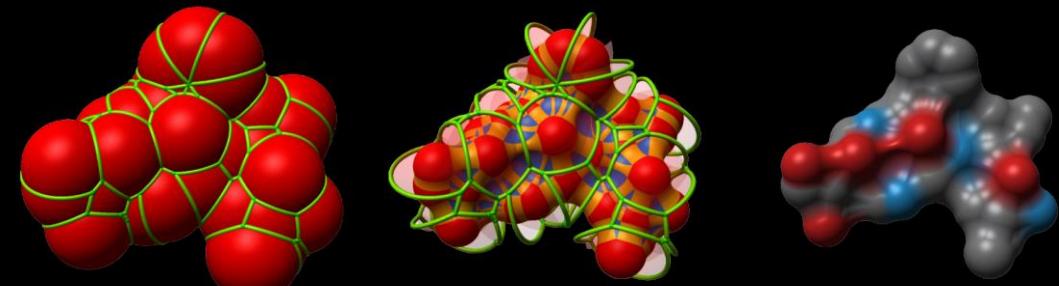
## Reduced Surface [SOS96]

- Efficient method
- But fully iterative so not parallelizable



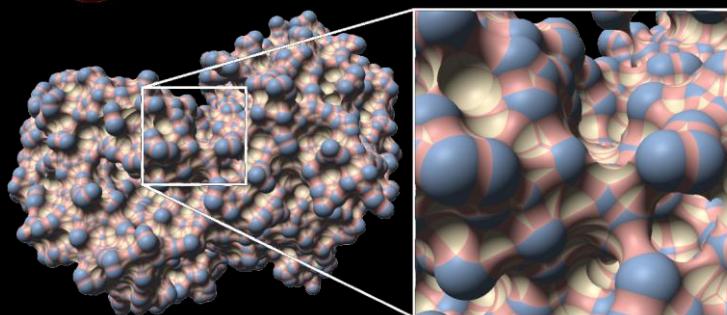
## Contour Build-up [TA96]

- Parallelizable on GPU [KGE11]
- Huge memory consumption (60k atoms: 5GB)



## Recent method [SK19]

- Less memory (60k atoms: 0,46GB)
- But slow...



[SOS96] Sanner M., et al. – [Reduced Surface: An efficient way to compute molecular surfaces](#) – Biopolymers – 1996

[TA96] Totrov M., Abagyan R. – [The contour-buildup algorithm to calculate the analytical molecular surface](#) – PLOS ONE – 1996

[KGE11] Krone M. et al. – [Parallel contour buildup algorithm for the molecular surface](#) – IEEE Bio. Data Vis. – 2011

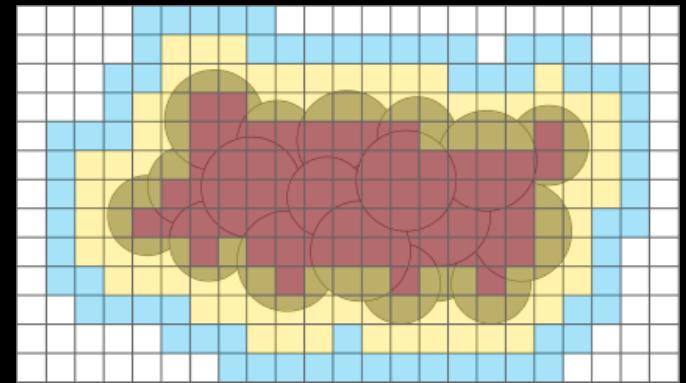
[SK19] Schäpfer M., Krone M. – [A Massively Parallel CUDA Algorithm to Compute and Visualize the Solvent Excluded Surface \[...\]](#) – MolVA – 2019

# SES construction: discrete approaches

Surface approximated by discretizing  $\mathbb{R}^3$

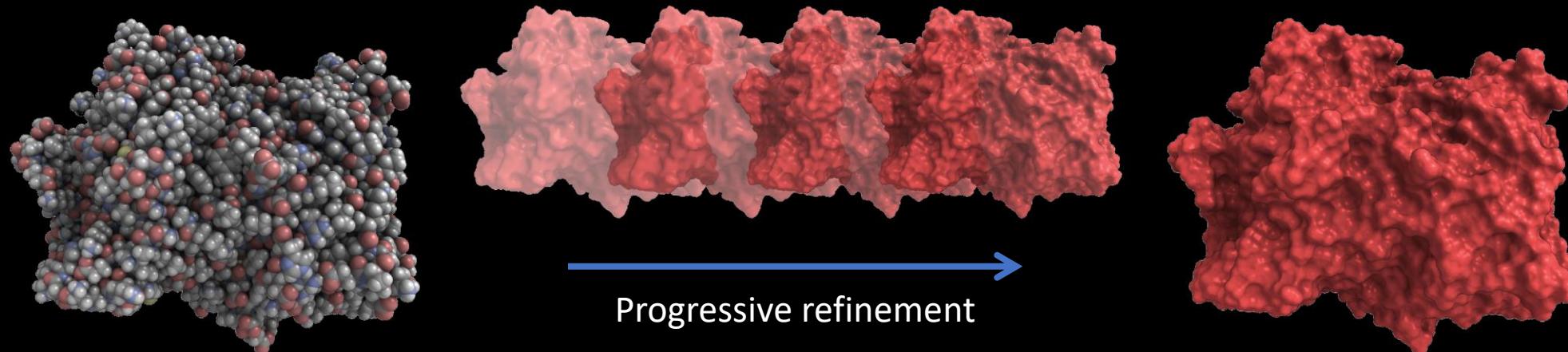
- Voxelisation representing a distance field

Surface extracted with Marching Cube



State-of-the-art method [HKG17]: progressive grid refinement

- Fast CUDA implementation (150 FPS, 500k atoms, GTX970, 720p)
- Quality limited by the grid size

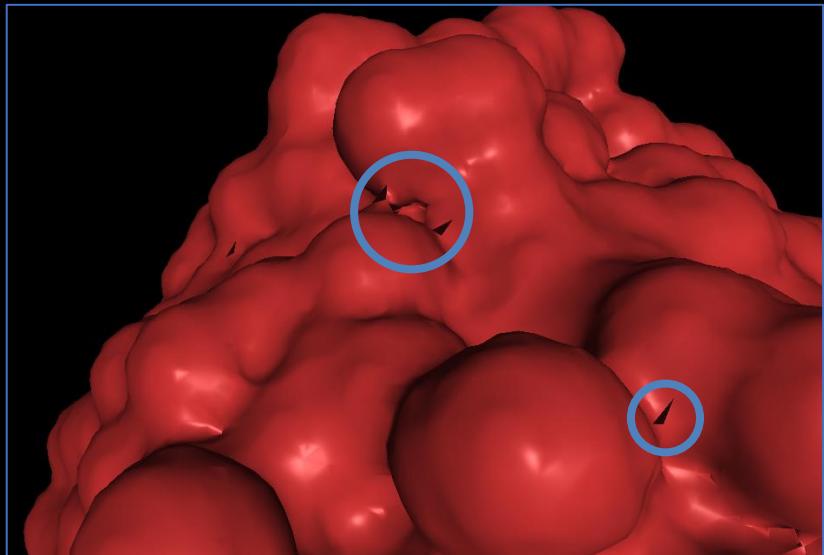
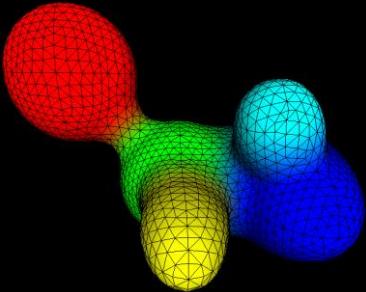


[HKG17] Hermosilla P., et al. – Interactive GPU-based Generation of Solvent Excluded Surfaces – CGI – 2017

# SES rendering

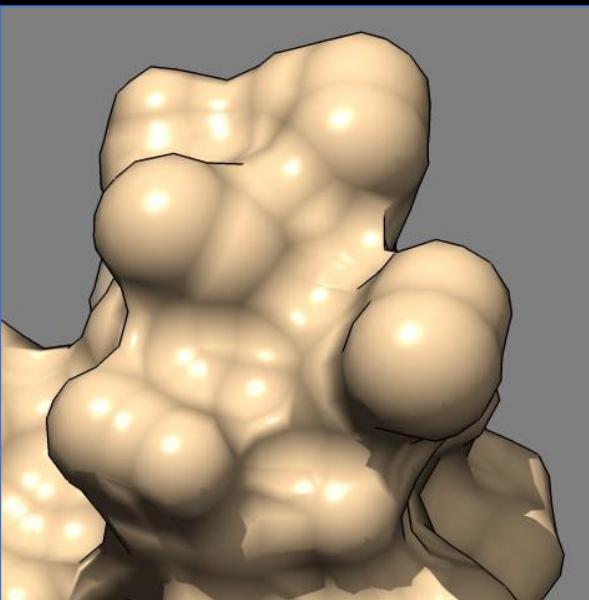
## With triangle meshes

- Huge memory consumption
- Numerical instability
- Quality depending on the number of triangles
- More triangles = slower

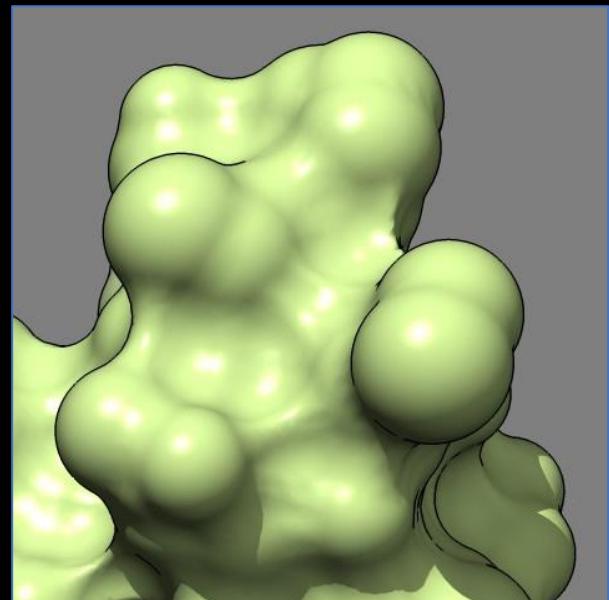


## With implicit surfaces (meshless)

- Few memory
- Pixel-perfect rendering
- Quite fast



VS



# Our approach

Part of C. Plateau—Holleville’s PhD thesis (started in October 2021)

Based on Quan and Stamm’s mathematical definition [QS16]

- Collaboration with B. Stamm (Stuttgart, Germany)

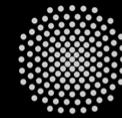
“Perfect” SES construction:

- Analytical
- Geometric singularities implicitly handled (no post-process)
- Computes the whole surface (even inside)

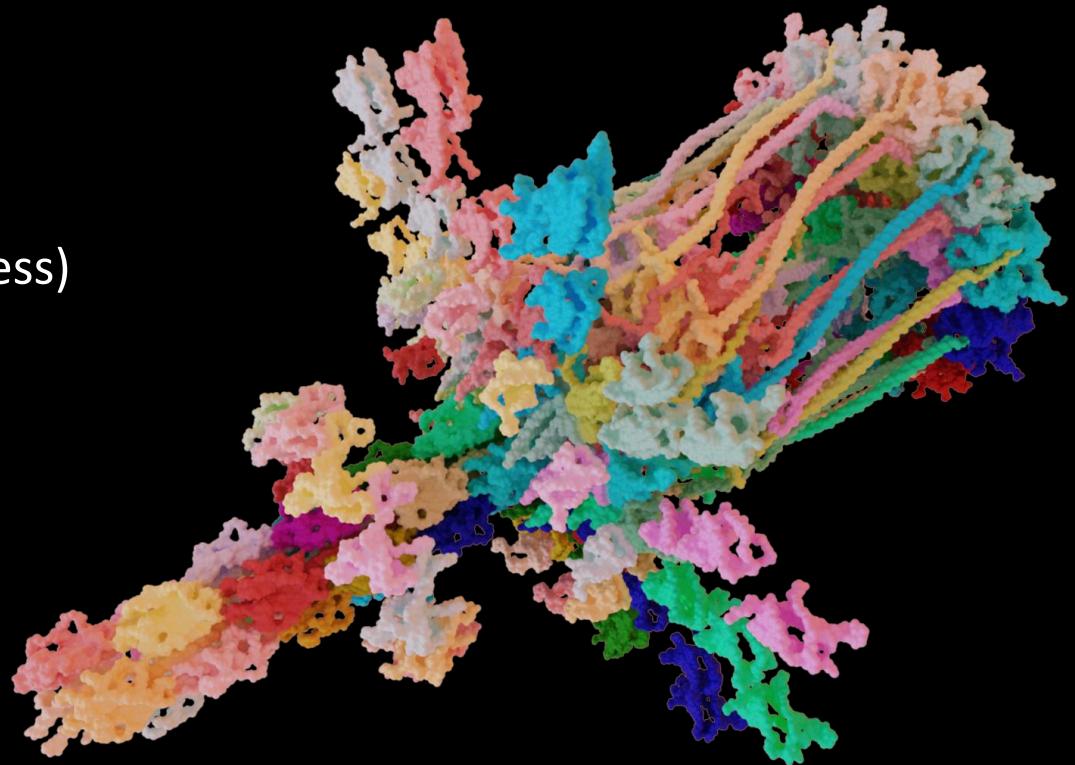
Rendering:

- Meshless ray-tracing (sphere-tracing)

To appear in IEEE TVCG (2024)



**University of Stuttgart**  
Institute of Applied Analysis and Numerical  
Simulation



[QS16] Quan C., Stamm B. – Mathematical Analysis and Calculation of Molecular Surfaces – Journal of Computational Physics – 2016

# Our contributions in a nutshell

A new algorithm/data structure to construct the SES

- Full surface (both interior and exterior)

Entirely parallelized on the GPU

- Cooperative intra-warp work

Compact in memory

- “Compute-over-store” strategy

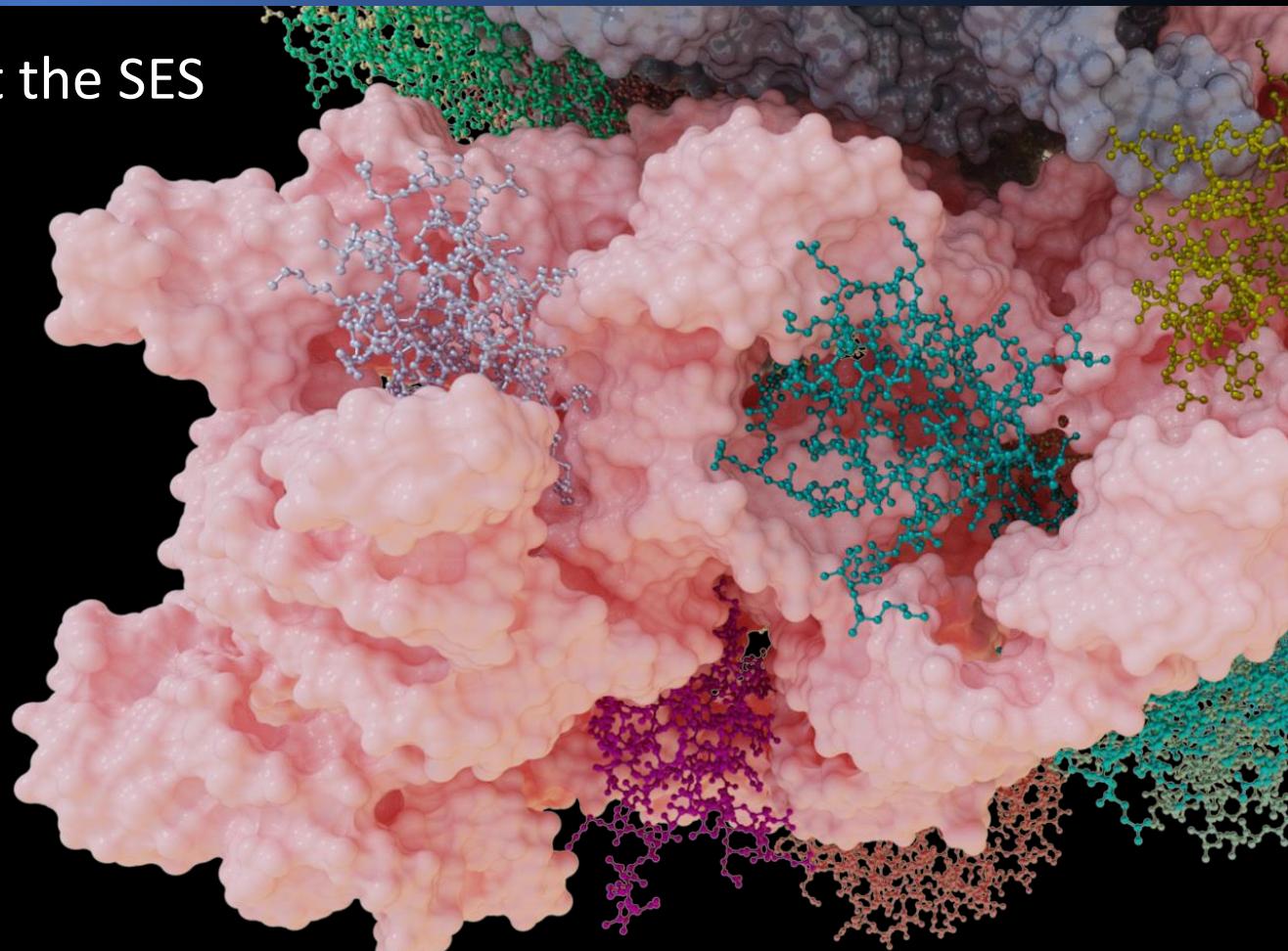
Directly utilizable for rendering

- Use of SDF/sphere tracing → pixel perfect

Outperform Contour-Buildup (CB) [\[KGE11\]](#)

- Most used method nowadays

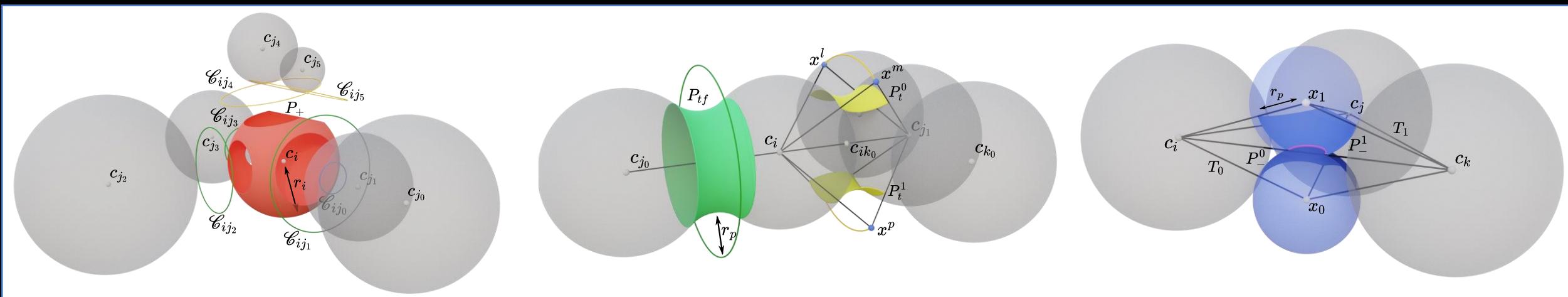
Open-source implementation



[KGE11] Krone M. et al. – Parallel contour buildup algorithm for the molecular surface – IEEE Bio. Data Vis. – 2011

# Geometric definition

Three kinds of geometric primitives (patches) [QS16]



Convex patches ( $P_+$ )

Toroidal patches ( $P_t, P_{tf}$ )

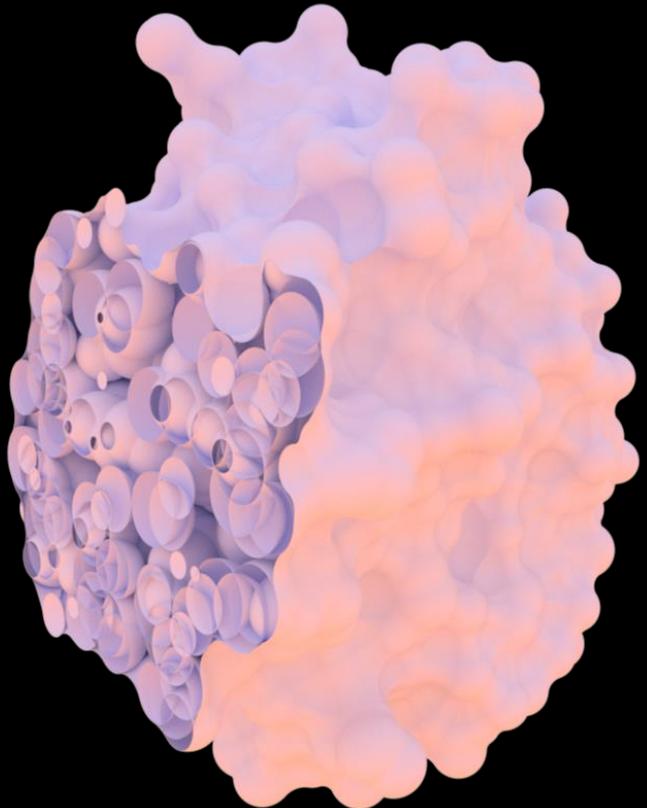
Concave patches ( $P_-$ )



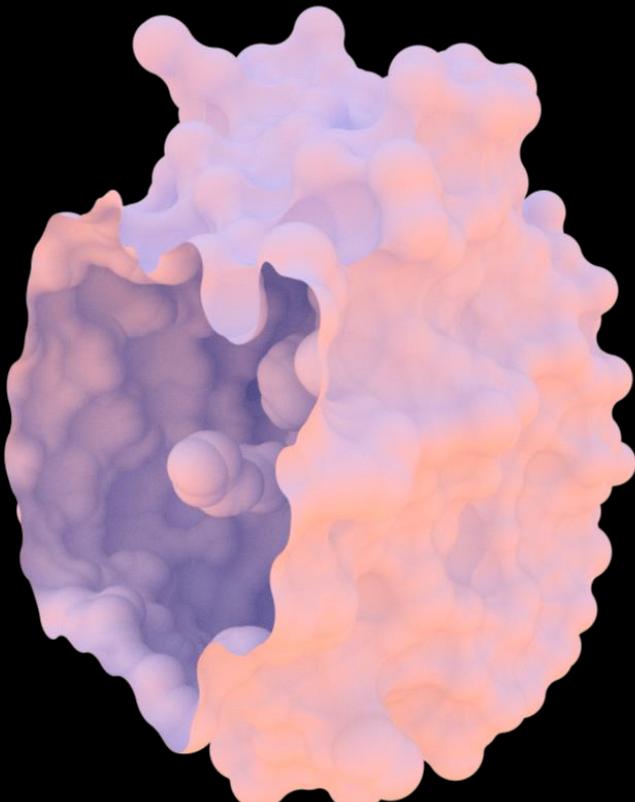
[QS16] Quan C., Stamm B. – Mathematical Analysis and Calculation of Molecular Surfaces – Journal of Computational Physics – 2016

# Complete surface computation

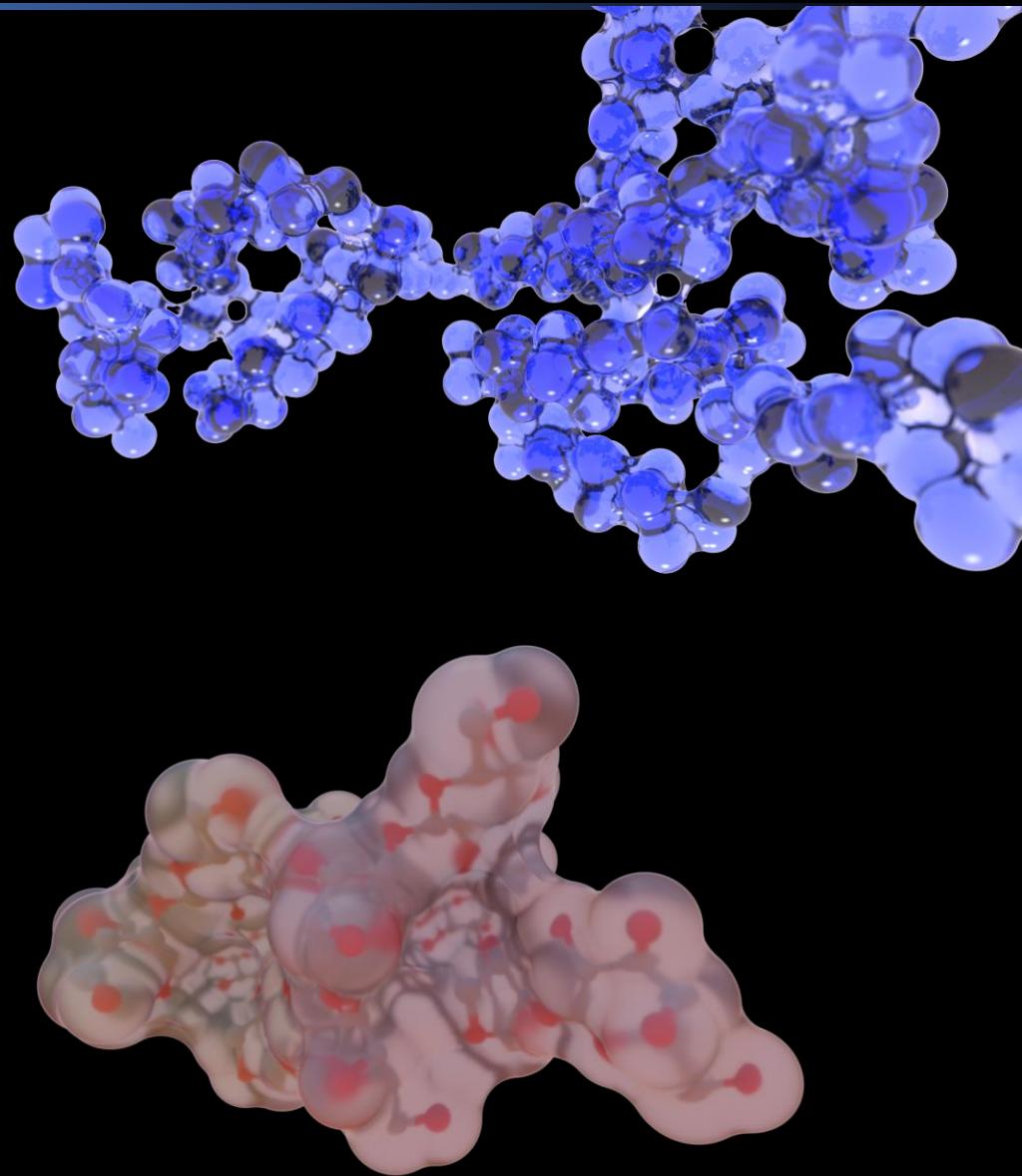
Useful e.g. for transparent rendering



Exterior surface



Complete surface



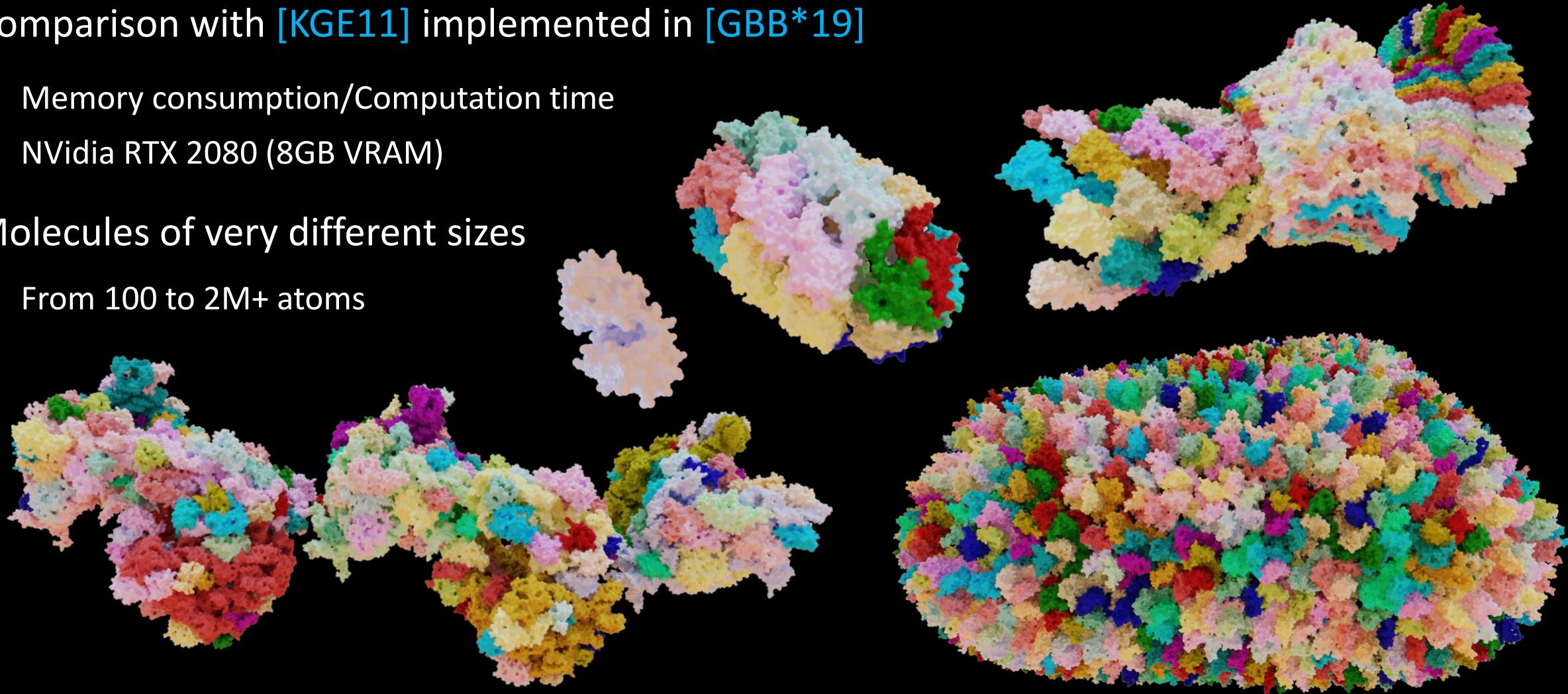
# Test setup

Comparison with [KGE11] implemented in [GBB\*19]

- Memory consumption/Computation time
- NVidia RTX 2080 (8GB VRAM)

Molecules of very different sizes

- From 100 to 2M+ atoms

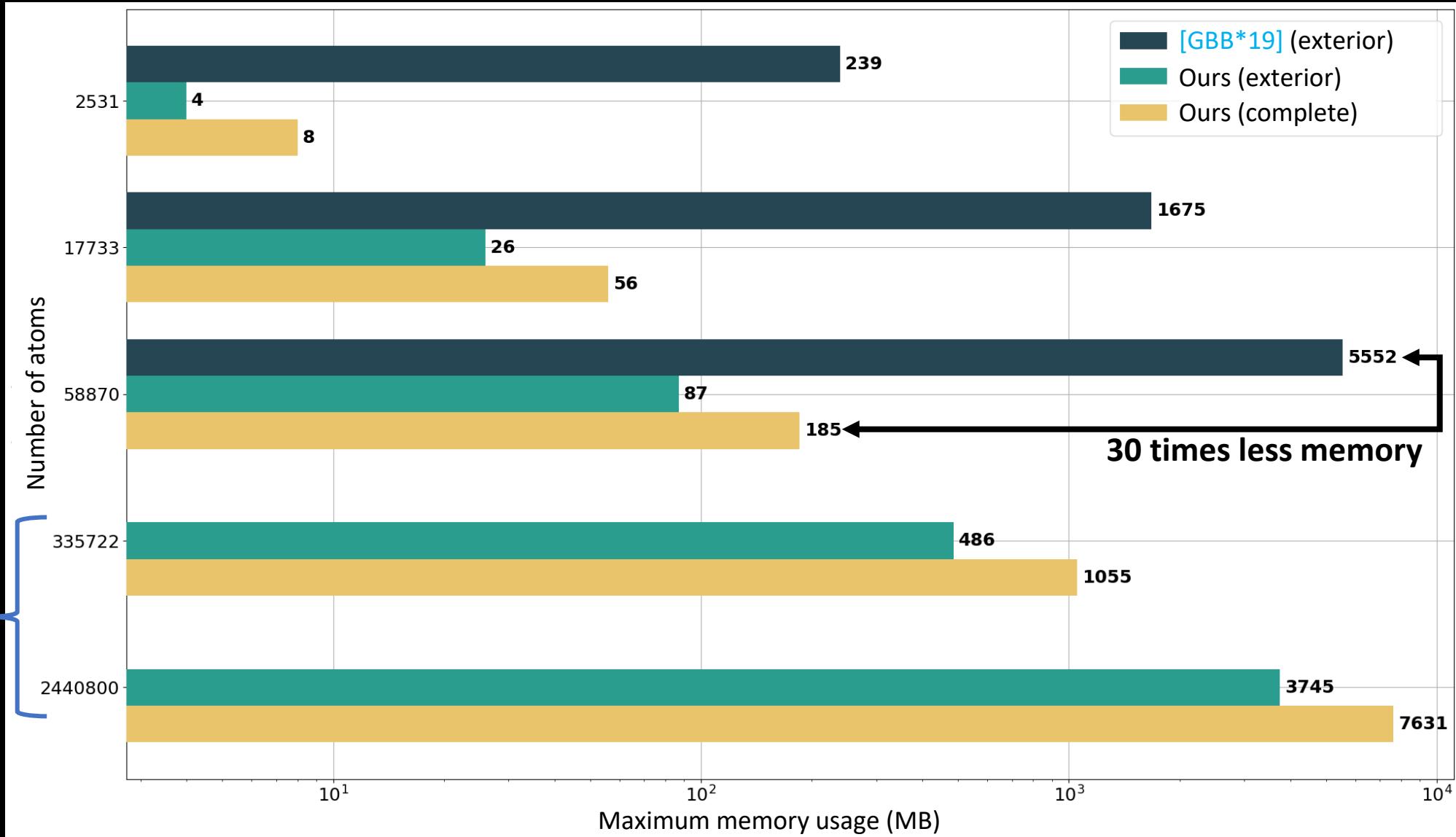


[KGE11] Krone M. et al. – Parallel contour buildup algorithm for the molecular surface – IEEE Bio. Data Vis. – 2011

[GBB\*19] Gralka et al. – Megamol – A comprehensive Prototyping Framework for Visualizations – The European Journal of Physics – 2019

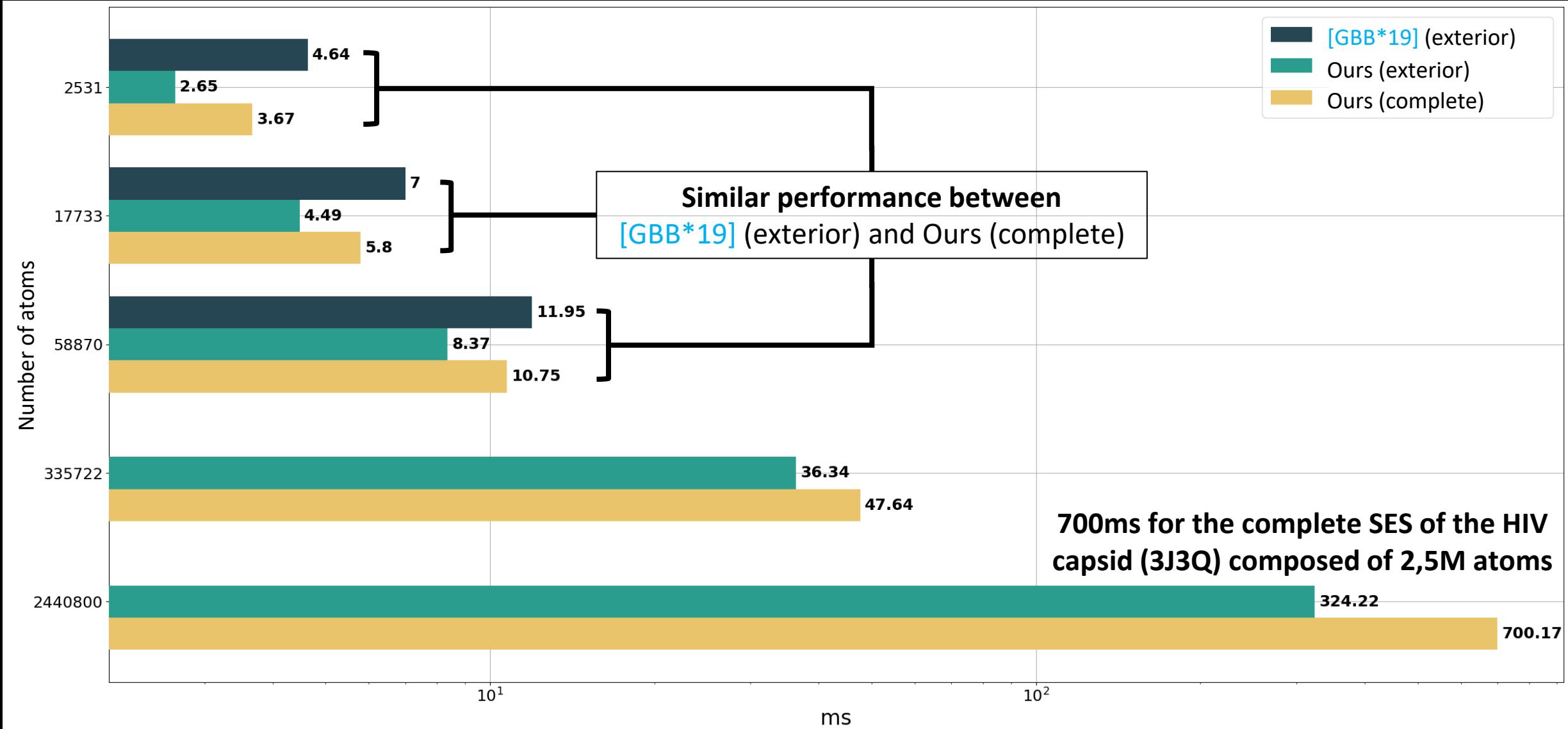
# Comparison with CB (Megamol [GBB\*19]): Memory (Nvidia RTX2080)

Less memory  
=  
More atoms!



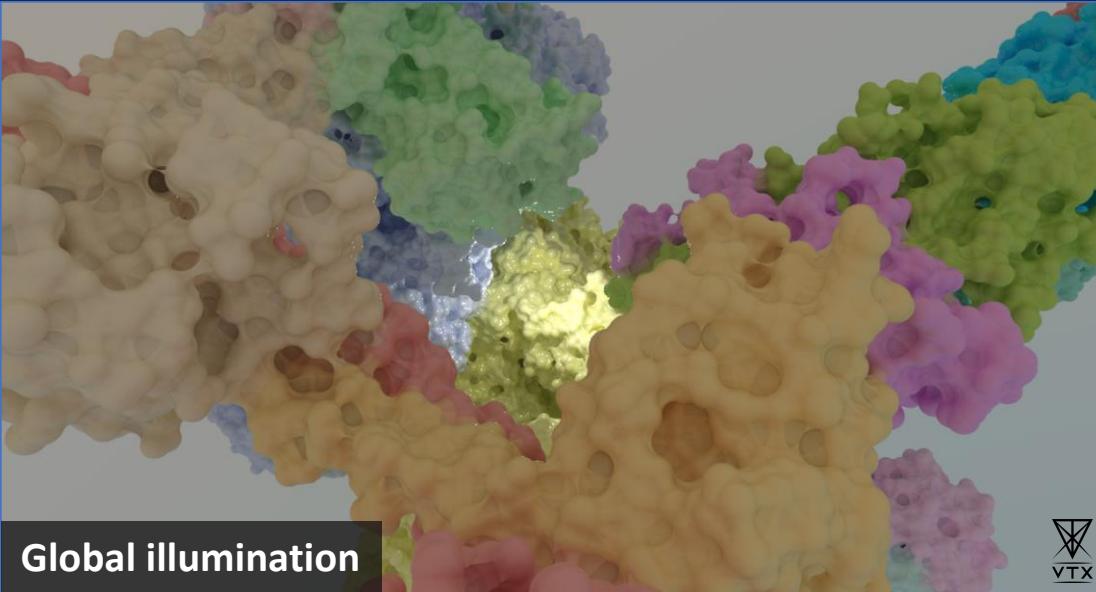
[GBB\*19] Gralka et al. – Megamol – A comprehensive Prototyping Framework for Visualizations – The European Journal of Physics – 2019

# Comparison with CB (Megamol [GBB\*19]): Time (NVidia RTX2080)

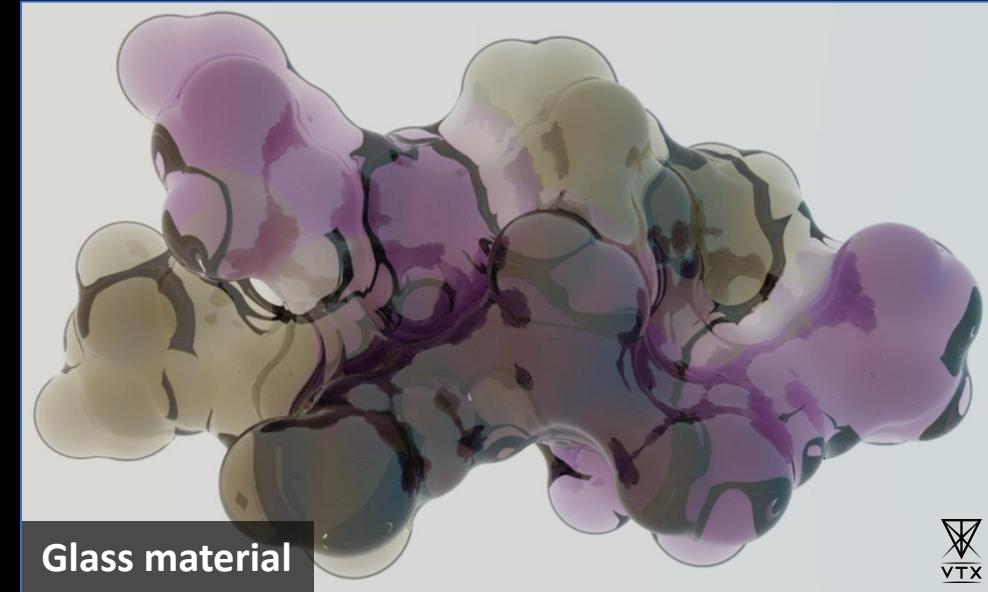


[GBB\*19] Gralka et al. – Megamol – A comprehensive Prototyping Framework for Visualizations – The European Journal of Physics – 2019

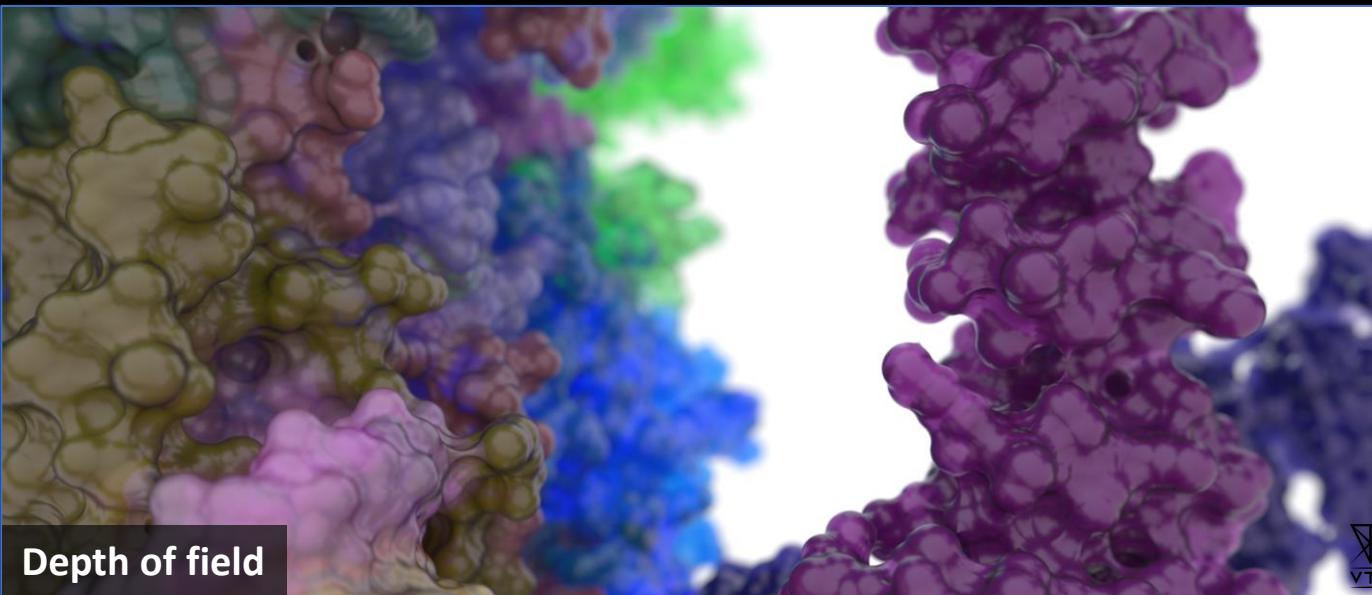
# More rendering results: molecules can be beautiful 😊



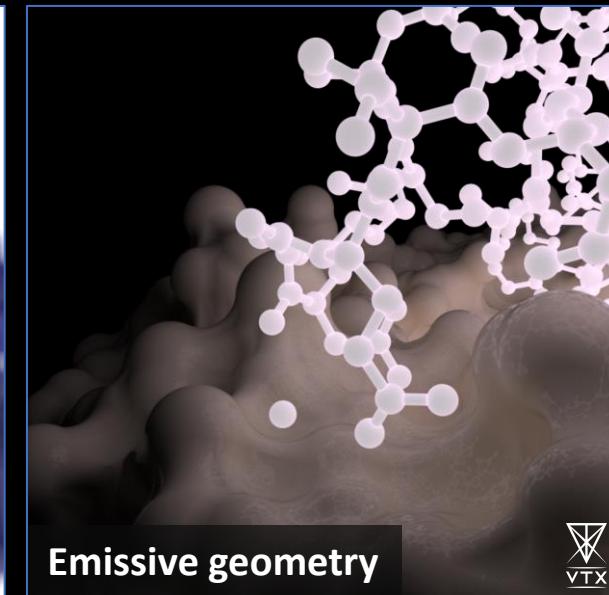
Global illumination



Glass material



Depth of field



Emissive geometry

# Limits and perspectives

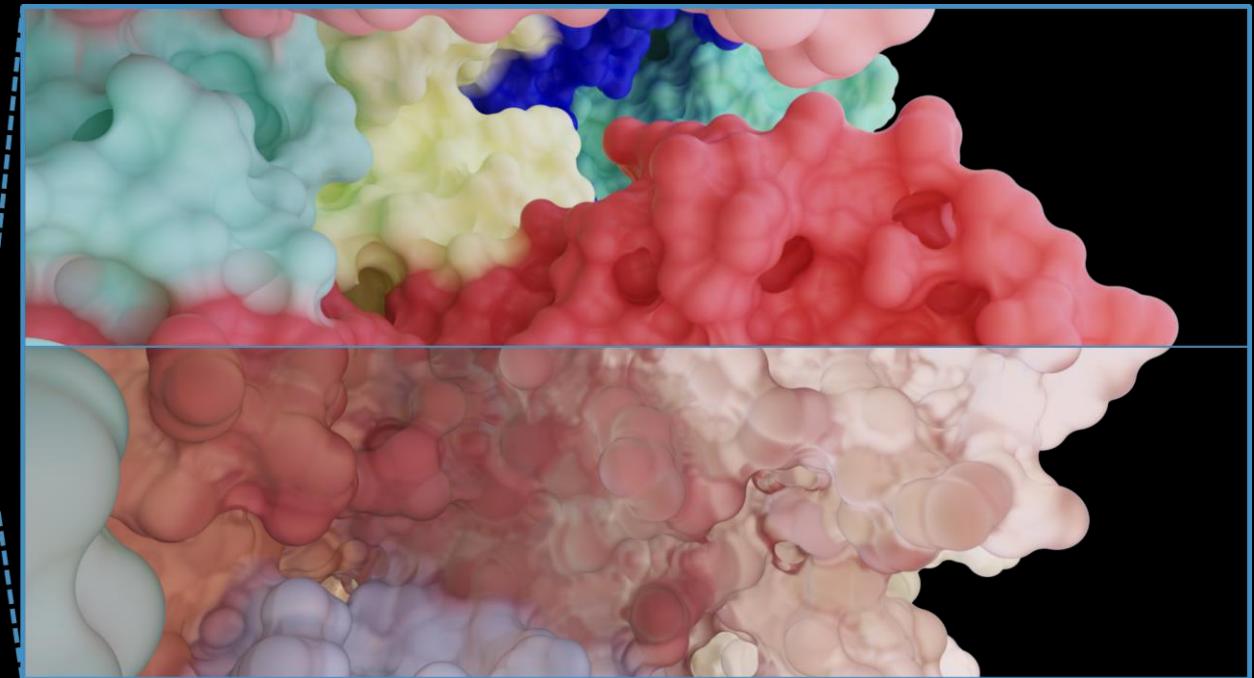
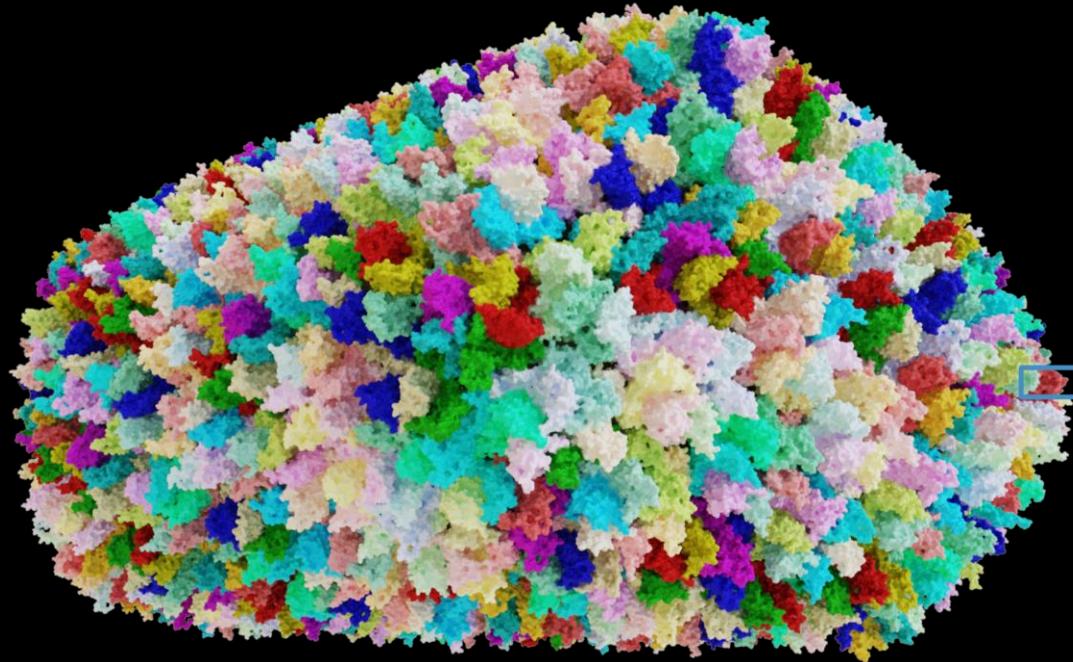
We can further reduce the computing charge

⇒ Finer space classification

For now, we need to recompute all the surface when the probe radius change

⇒ Reuse some computation

Release with VTX v1.0 (I hope soon!)



# What do we do in Limoges?

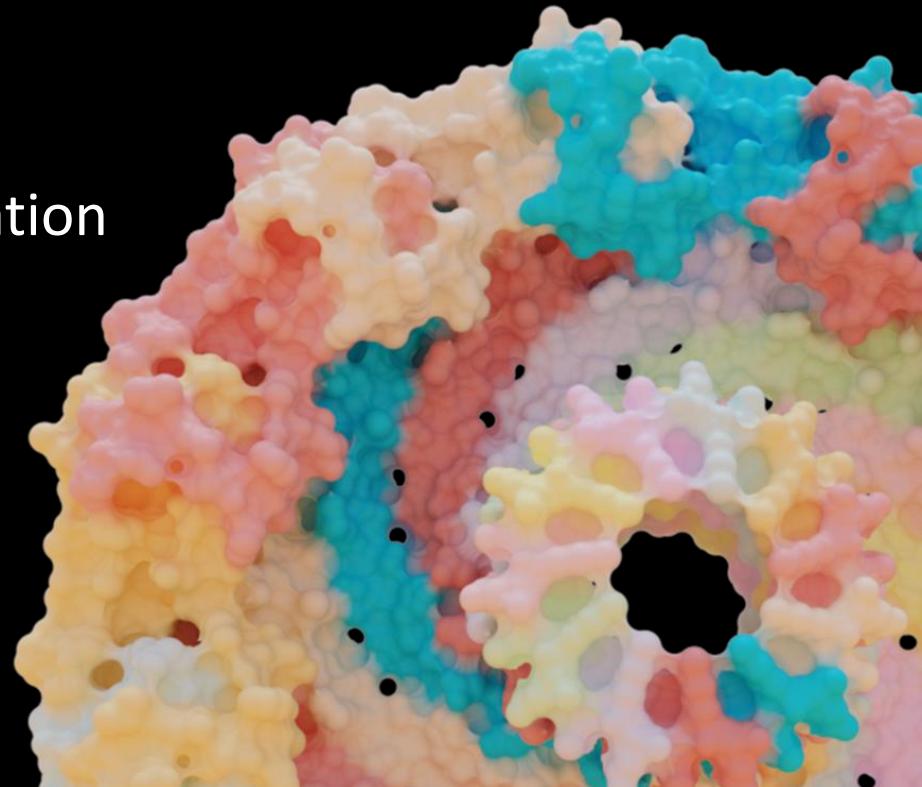
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# Voronoi diagram

Space partition of  $\mathbb{R}^d$  from a set of points  $P = \{p_0, p_1, \dots, p_n\}$  (seeds)

Each subspace  $V(p_i)$  (Voronoi cell) contains all the point in  $\mathbb{R}^d$  closer to  $p_i$  than to any other

$$V(p_i) = \{x \in \mathbb{R}^d \mid d(x, p_i) \leq d(x, p_j), \forall i \neq j\}$$

with  $d(x, p_i) = \|x - p_i\|$ , the Euclidean distance.

Useful in many applications *e.g.*:

- Meshing (Delaunay triangulation is the dual in  $\mathbb{R}^2$ )
- Clustering data
- ...

# Voronoi, Power and Apollonius diagrams

## Voronoi diagram

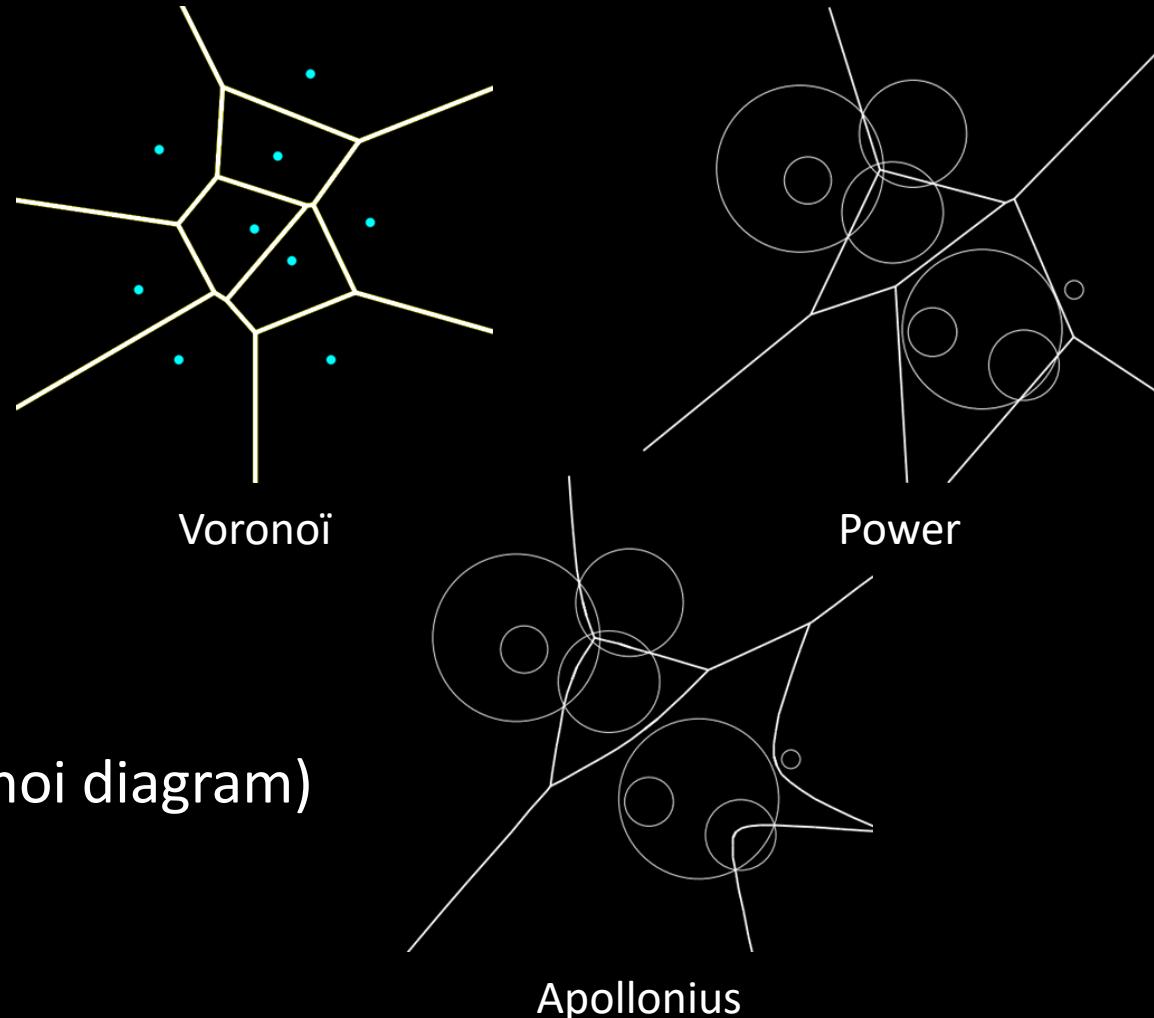
- Seeds:  $p \in \mathbb{R}^d$
- Euclidean distance:  $d(x, p_i) = \|x - p_i\|$

## Power diagram

- Weighted seeds:  $s = (p \in \mathbb{R}^d, r \in \mathbb{R}^+)$
- Power distance:  $\delta^{(2)}(x, s_i) = \|x - p_i\|^2 - r_i^2$

## Apollonius diagram (or Additively Weighted Voronoi diagram)

- Weighted seeds:  $s = (p \in \mathbb{R}^d, r \in \mathbb{R}^+)$
- Distance to the sphere:  $\delta(x, s_i) = \|x - p_i\| - r_i$
- “Voronoi diagram of spheres/balls”



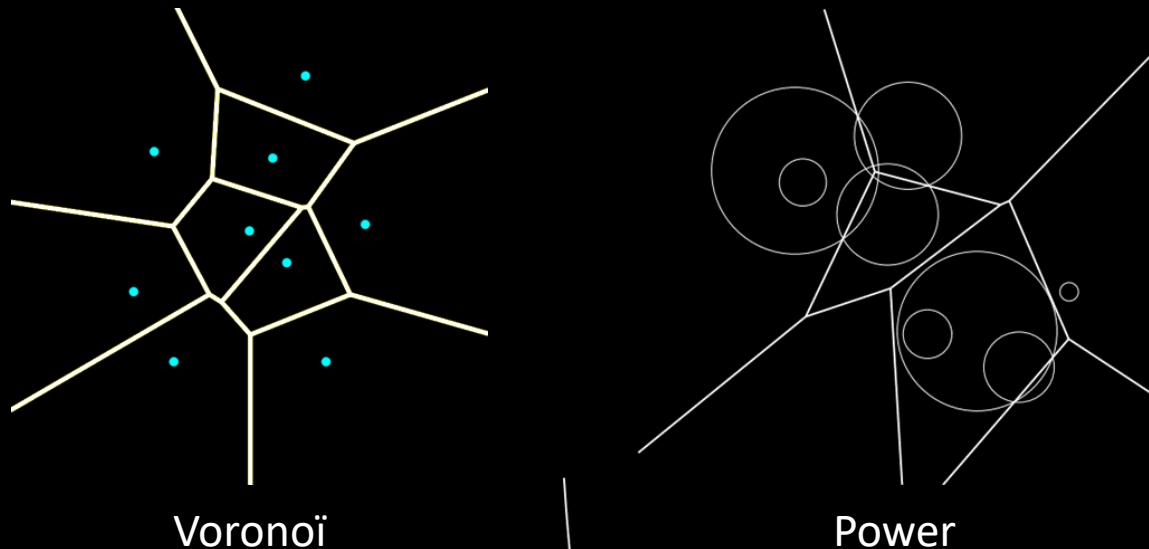
Illustrations from [BWY07]

[BWY07] Boissonnat D. et al. – Curved Voronoi Diagrams – Effective Computational Geometry for Curves and Surfaces – 2007

# Voronoi, Power and Apollonius diagrams

## Voronoi diagram

- Seeds:  $p \in \mathbb{R}^d$
- Euclidean distance:  $d(x, p_i) = \|x - p_i\|$



## Power diagram

- Weighted seeds:  $s = (p \in \mathbb{R}^d, r \in \mathbb{R}^+)$
- Power distance:  $\delta^{(2)}(x, s_i) = \|x - p_i\|^2 - r_i^2$

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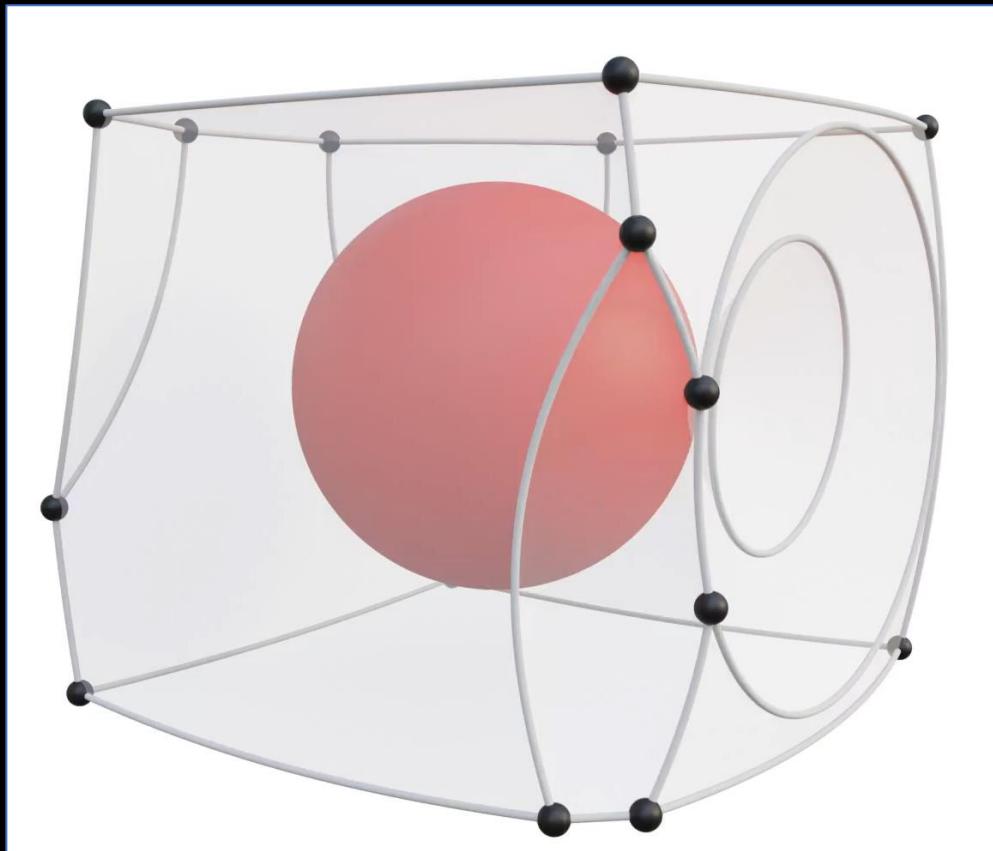
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- Distance to the sphere:  $\delta(x, s_i) = \|x - p_i\| - r_i$
- “Voronoi diagram of spheres/balls”

Illustrations from [BWY07]

# Apollonius diagram

Harder to compute than Voronoï or Power diagram

- Facets (bisectors) of a cell can be curved and topologically disconnected



# Apollonius diagram computation

Few publicly available implementation

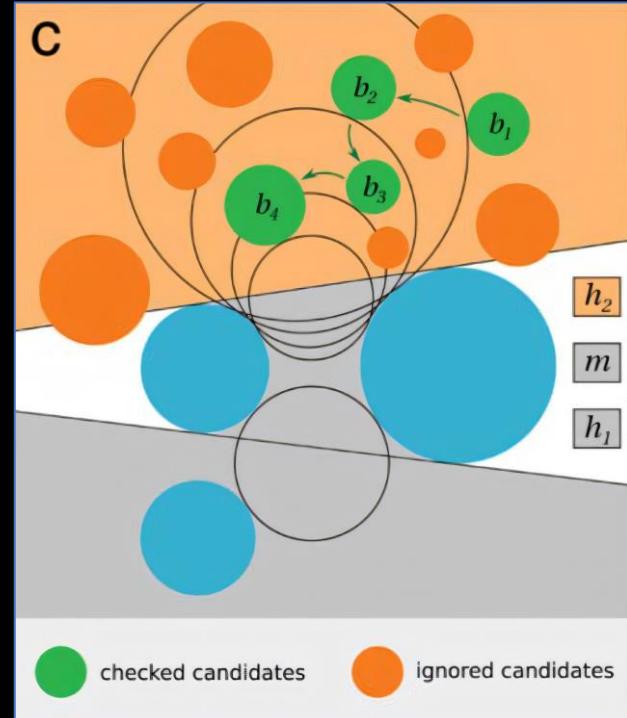
- Voronota [OK14] / AwVoronoi [AwV]

Main algorithm: Edge-Tracing [KCK05]

- Easy to implement but not robust and purely sequential

Slower alternatives or without implementation in  $\mathbb{R}^3$

- Predicates analysis [Kam20]
- Space exploration [WYM\*20]
- Topology based [LSK22]



Edge-Tracing [OK14]

[OK14] Olechnovič K. et al – [Voronota: A fast and reliable tool for computing the vertices of the Voronoi \[...\]](#) – J. of Computational Chemistry – 2014

[AwV] Maňák M. et al. – [AwVoronoi](#) – <http://awvoronoi.sf.net> – accessed on March 2024

[SLF\*11] Secord A. et al. – [Perceptual Models of Viewpoint Preference](#) – ACM Transactions on Graphics – 2011

[Kam20] Kamarianakis M. – [Predicates of the 3D Apollonius Diagram](#) – arXiv – 2020

[WYM\*20] Wang P. et al. – [Robust Computation of 3D Apollonius Diagrams](#) – Computer Graphics Forum – 2020

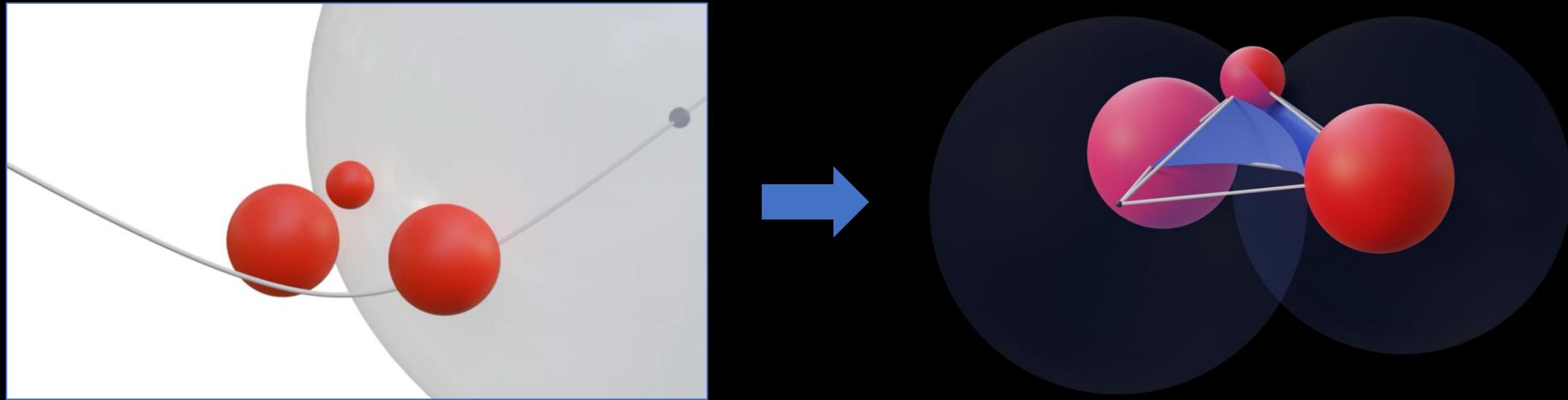
[LSK22] Lee M., et al. – [Robust Construction of Voronoi Diagrams of Spherical Balls in Three-Dimensional Space](#) – Computer Aided Design – 2022

# Link between the SES and the Apollonius diagram

Apollonius like a generalization of the SES

- Regardless the probe size ( $r_p \in [0, +\infty[$ )
- Contains all possible probe positions for a given configuration

Construct the SES from the Apollonius diagram [RDY\*05, MJK16]



[RDY\*05] Ryu J. et al. – [Computation of Molecular Surface Using Euclidean Voronoi Diagram](#) – Computer Aided Design – 2005

[MJK16] Maňák M. et al. – [Interactive Analysis of Connolly Surfaces for Various Probes](#) – Computer Graphics Forum – 2016

# Our work

Continuation of C. Plateau--Holleville's PhD thesis

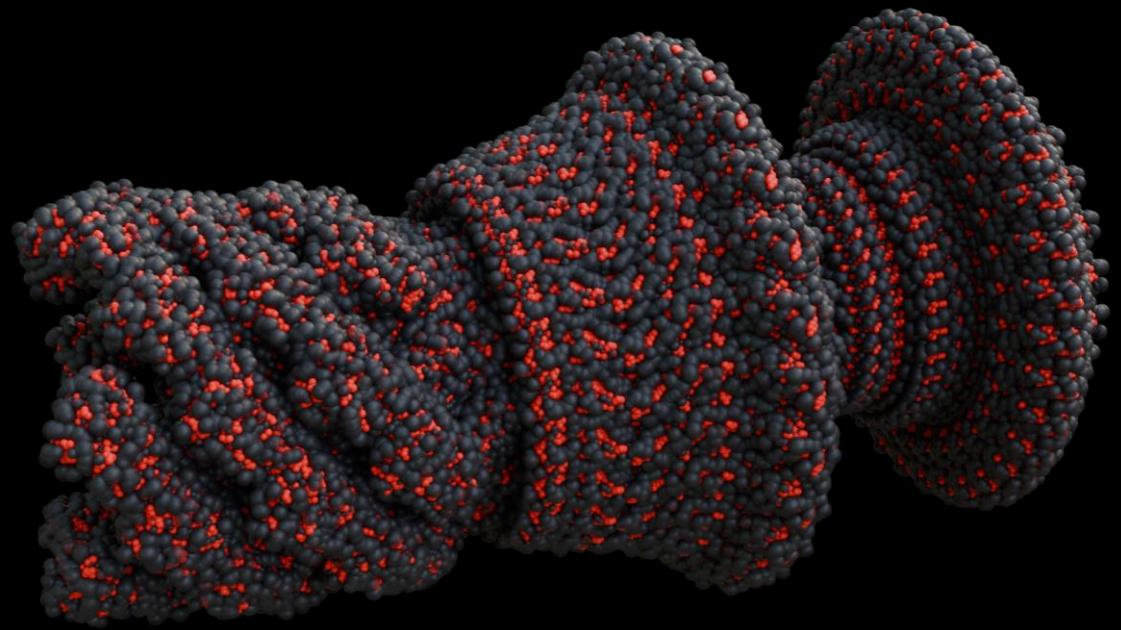
New robust and fast method to compute Apollonius diagram

Application to molecular scenes:

- SES computation
- Cavity detection

Two parts job:

- Mathematical analysis and characterization
- Efficient GPU parallel implementation



# Mathematical analysis and characterization

A lot of equations... 😅

C. Plateau-Holleville et al. / Journal of Computational Physics 00 (2024) 1–14  
describing  $\Pi_{ijk}^2 = \Pi_{ij}^2 \cap \Pi_{ik}^2$  through the parameter  $\hat{x}$ .  
The intersection with the cone  $\Gamma_i$  can then be expressed based on the given parametrization of  $\Pi_{ijk}^2$ , yielding

$$\begin{cases} x_d = d_1 - C_{1\bullet}\hat{x} \\ x_{d+1} = d_2 - C_{2\bullet}\hat{x} \\ \sum_{i=1}^{d-1} (x_a - p_{i,d})^2 + (x_d - p_{i,d})^2 = (x_{d+1} + r_i)^2. \end{cases}$$

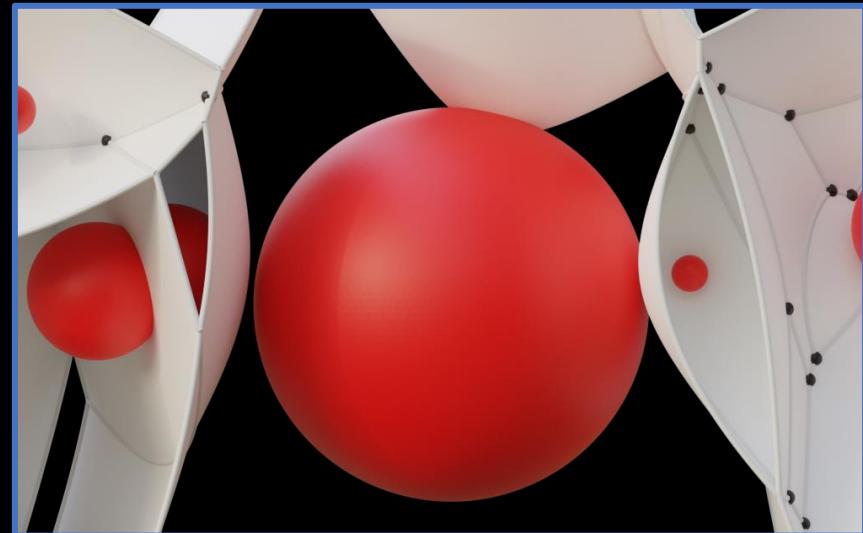
Let  $x' = (x_1 - p_{1,1} \quad \dots \quad x_d - p_{d,d} \quad x_{d+1} + r_i)^T$ , with  $x' = x - p_i$  and  $x = x' + p_i$  then, by expressing the system relatively to  $s_i$  based on  $x'$ , we obtain

$$\begin{cases} x'_d = x_d - p_{i,d} = d_1 - C_{1\bullet}\hat{x} - p_{i,d} = d_1 - C_{1\bullet}(\hat{x}' + \hat{p}_i) - p_{i,d} \\ x'_{d+1} = x_{d+1} + r_i = d_2 - C_{2\bullet}\hat{x} + r_i = d_2 - C_{2\bullet}(\hat{x}' + \hat{p}_i) + r_i \\ \sum_{i=1}^{d-1} x'_a^2 + x'_d^2 = x'_{d+1}^2 \\ \sum_{i=1}^{d-1} x_a^2 + x_d^2 = x_{d+1}^2. \end{cases}$$

Based on these changes, the last two coordinates of  $\Pi_{ij}^2 \cap \Pi_{ik}^2$  can now be inserted into the equation of  $\Gamma_i$  giving

$$\begin{aligned} & \| \hat{x}' \|^2 + (e_1 - C_{1\bullet}\hat{x}')^2 = (e_2 - C_{2\bullet}\hat{x}')^2 \\ & \Leftrightarrow \| \hat{x}' \|^2 + e_1^2 - 2e_1 C_{1\bullet}\hat{x}' + (C_{1\bullet}\hat{x}')^2 = e_2^2 - 2e_2 C_{2\bullet}\hat{x}' + (C_{2\bullet}\hat{x}')^2 \\ & \Leftrightarrow \| \hat{x}' \|^2 + \hat{x}' C_{1\bullet} C_{1\bullet}^T \hat{x}'^T - \hat{x}' C_{2\bullet} C_{2\bullet}^T \hat{x}'^T + 2(e_1 C_{2\bullet} - e_1 C_{1\bullet})\hat{x}' = e_2^2 - e_1^2 \\ & \quad \hat{x}' E \hat{x}'^T + 2(e_2 C_{2\bullet} - e_1 C_{1\bullet})\hat{x}' = e_2^2 - e_1^2, \text{ with } E = I + C_{1\bullet} C_{1\bullet}^T - C_{2\bullet} C_{2\bullet}^T \\ & \Leftrightarrow \hat{x}' E \hat{x}'^T + 2M \hat{x}' = e_2^2 - e_1^2, \text{ with } M = e_2 C_{2\bullet} - e_1 C_{1\bullet}. \end{aligned}$$

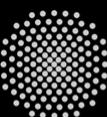
In  $\mathbb{R}^2$ , notice that  $\hat{x}', M \in \mathbb{R}$  resulting in the quadratic expression

$$E \hat{x}'^2 + 2M \hat{x}' - e_2^2 + e_1^2 = 0.$$


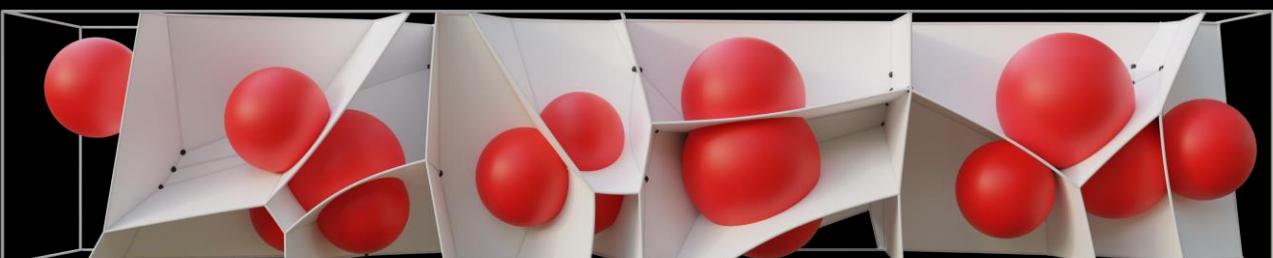
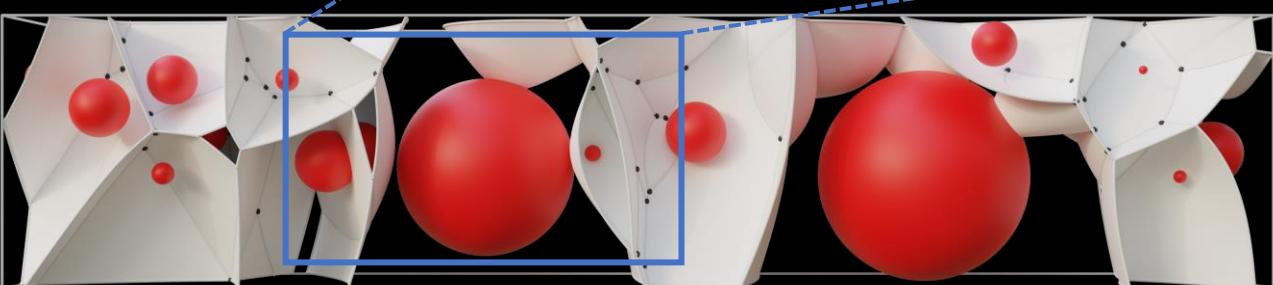
## Iterative construction process

- Brute force but robust
- Baseline for faster algorithm

Work with B. Stamm (Stuttgart, Germany)

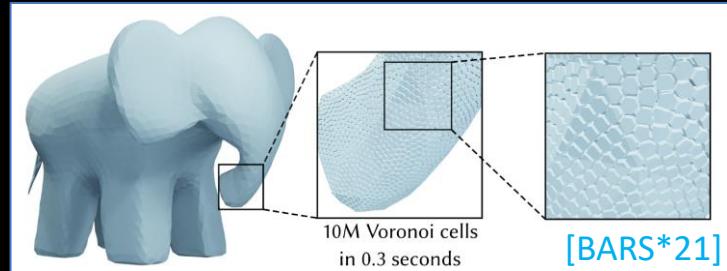
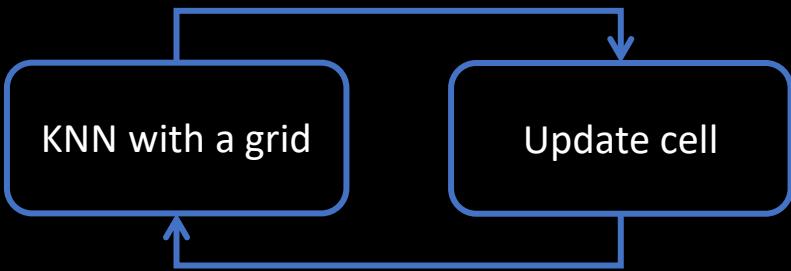


**University of Stuttgart**  
Institute of Applied Analysis and Numerical Simulation



# Efficient GPU implementation

State-of-the-art methods for Voronoï [RSLL18] and Power diagrams [BARS\*21]



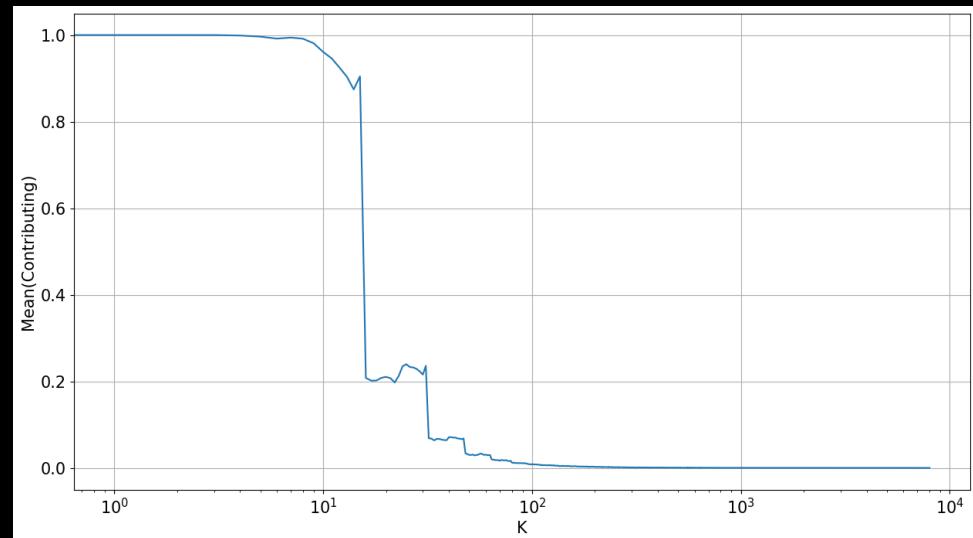
Not adapted for Apollonius...

- K should be high to get all the contributing neighbors
- A lot of seeds do not contribute at all

Design a new search strategy (hierarchical)

Work in progress (results promising):

- Goal = submit to SIGGRAPH Asia (may 2024)



Mean of contributing neighbors w.r.t K (for 50k atoms)

[RSLL18] Ray N. – Meshless Voronoï on the GPU – ACM Transactions On Graphics – 2018

[BARS\*21] Basselin J. et al. – Restricted Power Diagrams on the GPU – Computer Graphics Forum – 2021

# What do we do in Limoges?

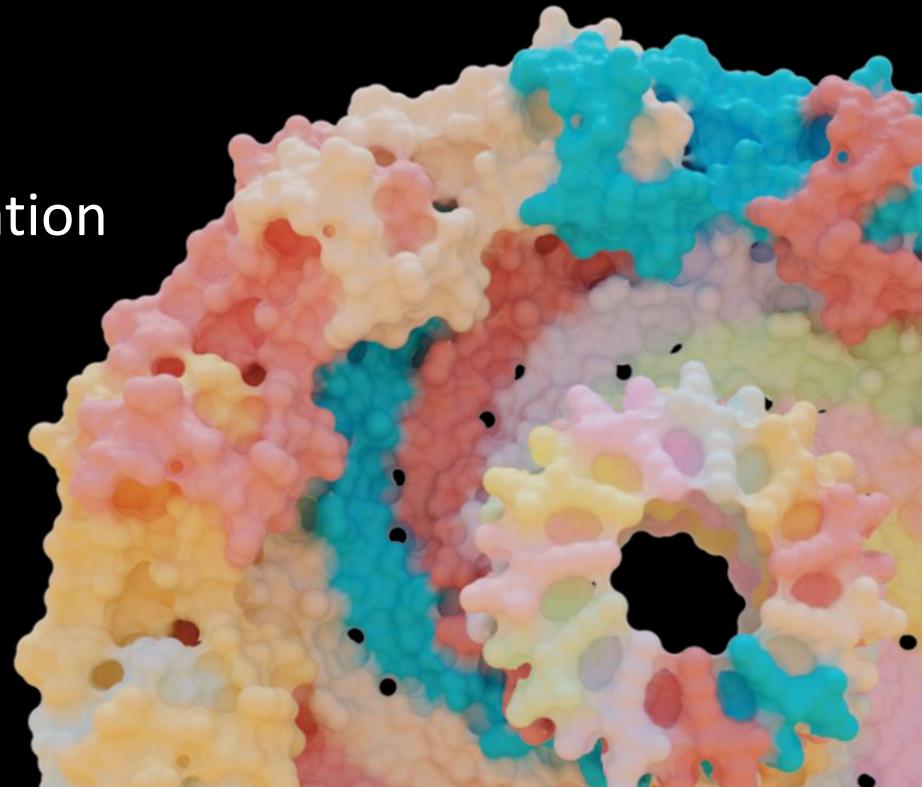
VTX: high-performance molecular visualization software

Efficient construction of Solvent Excluded Surface (SES)

Apollonius diagrams computation

Computer-aided generation of molecular simulation illustration

UDock2: Protein-protein docking



# Illustration of molecular simulations

Useful for researchers to share their results (with other experts or general public)

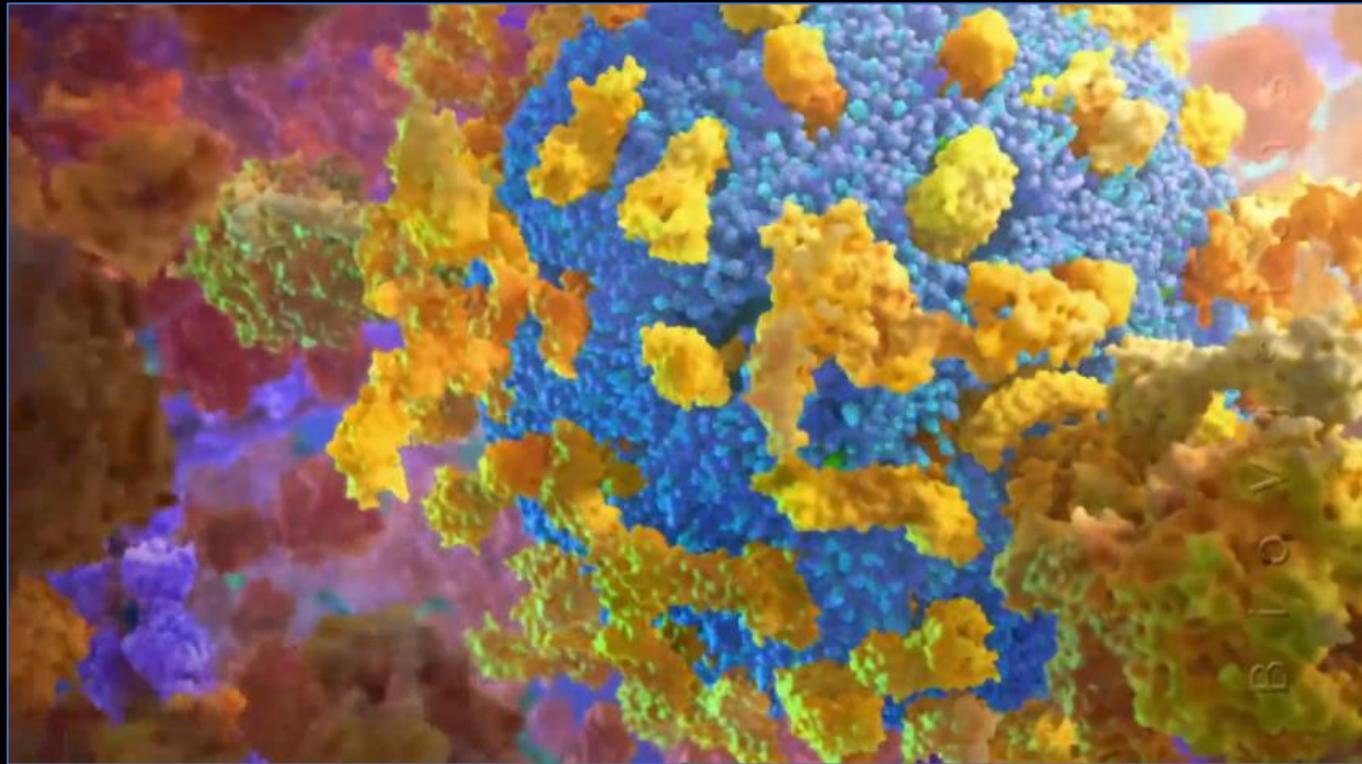
Molecular scenes are “chaotic”:

- Many atoms moving constantly
- No ground/no ceiling

Making good videos is hard...

- What do we want to see?
- How to ensure the object visibility?
- How to handle atoms movement?
- How to find a good camera trajectory?

Only few works on the topic



“Inner Life of a Cell” – Harvard University, USA  
Produced by a dedicated studio (XIVO Scientific Animation)

# Our work

PhD thesis of V. Larroque (started in January 2023)

- Also its master internship (5 months)
- Founded with Qubit Pharmaceuticals



Designing new methods to assist bio-chemical scientists to create illustrations of their work

For a single molecule:

- Automatic viewpoint selection
- Tour creation

For more complicated (dynamic) scenes:

- Camera trajectory
- Pathfinding

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# Related works for general objects

Viewpoint quality evaluation:

- Metric  $f(v)$  gives a score  $s$  from a viewpoint  $v$

Examples:

- *Projected surface* [PB96]: most of the object is visible
- *Viewpoint entropy* [VFSH01] based on Shannon's information theory: most informative viewpoint

$$f(\text{Dragon}) = \text{X} \quad f(\text{Dragon}) = \checkmark$$

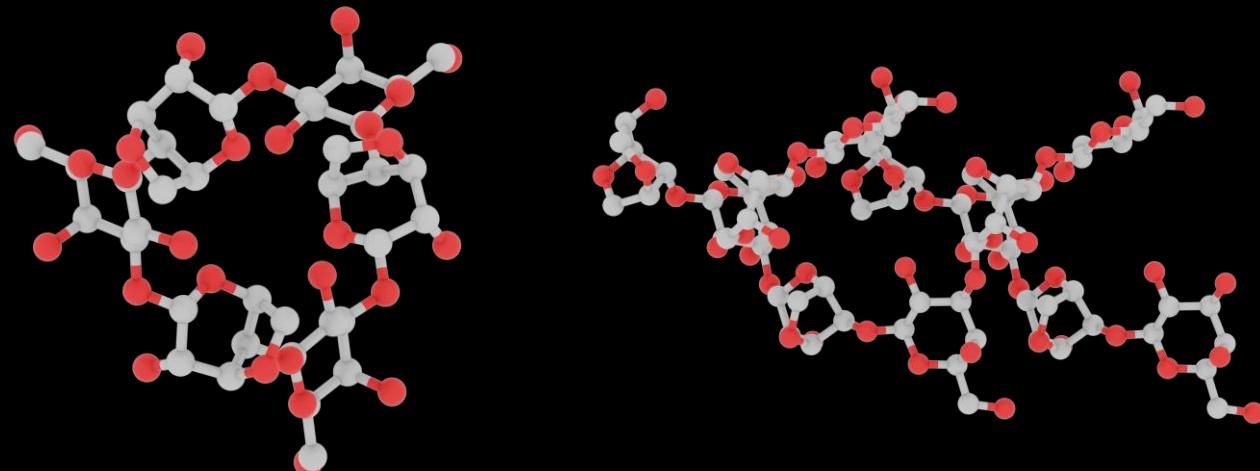
Two state-of-the-art [SLF\*11, BFS\*18]

- [PB96] Plemenos D. and Benayada M. – Intelligent Display in Scene Modeling. New Techniques to Automatically [...] – GraphiCon – 1996
- [VFSH01] Vázquez P.-P., et al. – Viewpoint Selection Using Viewpoint Entropy: Automatic View Selection – VMV Conference – 2001
- [SLF\*11] Secord A. et al. – Perceptual Models of Viewpoint Preference – ACM TOG – 2011
- [BFS\*18] Bonaventura X., et al. – A Survey of Viewpoint Selection Methods for Polygonal Models – Entropy – 2020

# Related works for molecules

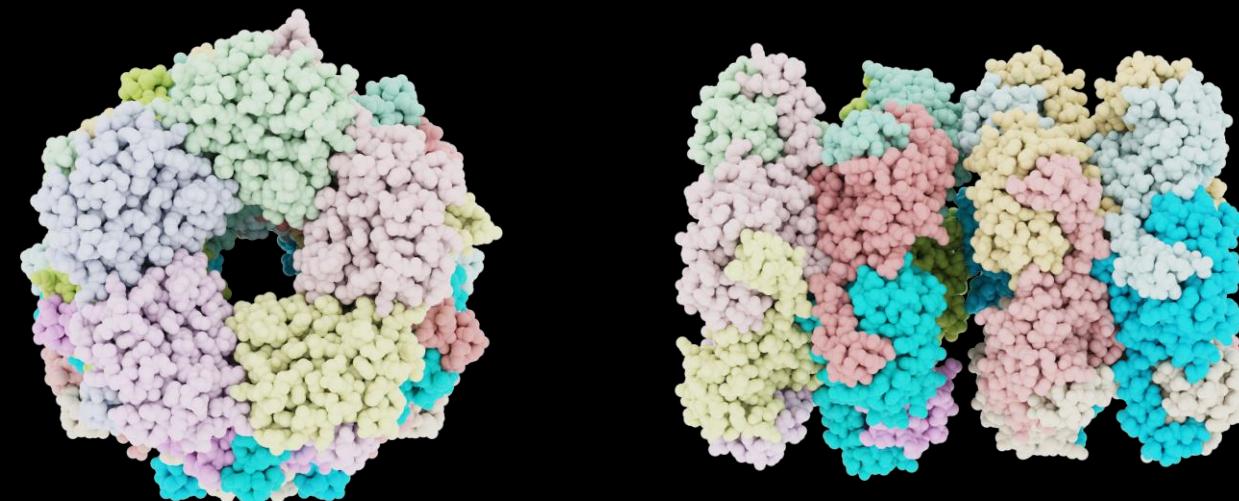
## Finding alignment [VFLS02]

- Adaptation of *Viewpoint entropy*



## Finding tunnels [HVH+16]

- Adaptation of [VFLS02]



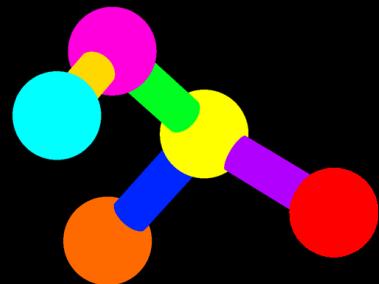
[VFLS02] Vázquez P.-P., et al. – Viewpoint entropy: a new tool for obtaining good views of molecules – VISSYM Conference – 2002

[HVH+16] Heinrich M. et al. – Evaluating Viewpoint Entropy for Ribbon Representation of Protein Structure – Computer Graphics Forum – 2016

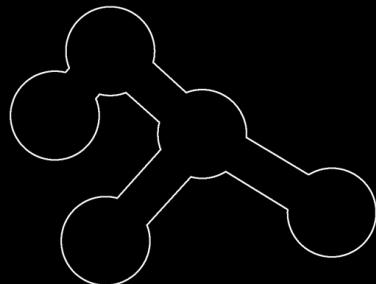
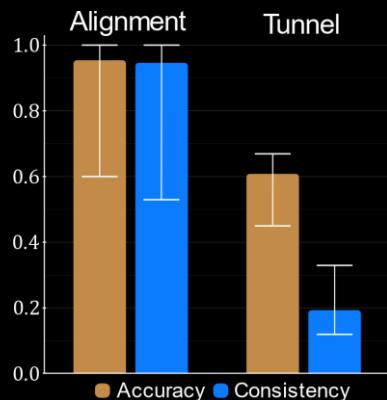
# Analysis of general metrics for molecules

Evaluation of 20 metrics from [SLF\*11, BFS\*18] classified into 5 categories:

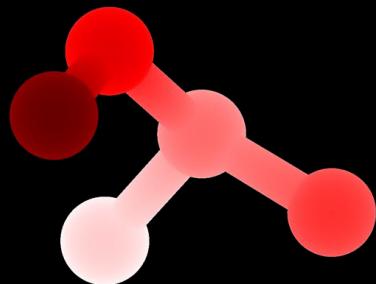
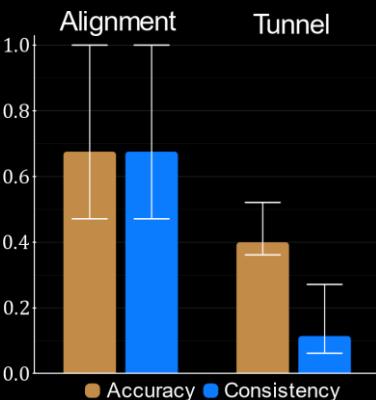
- How efficient they are to find alignment and/or tunnels?



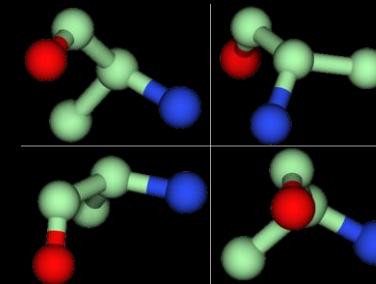
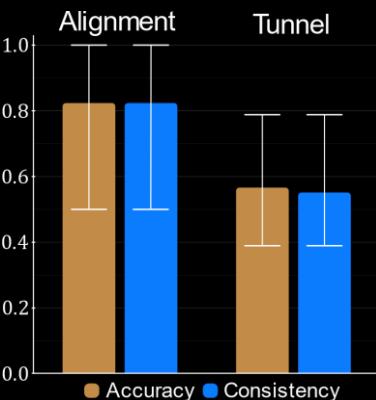
Surface (9)



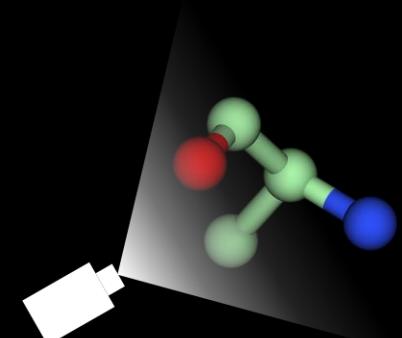
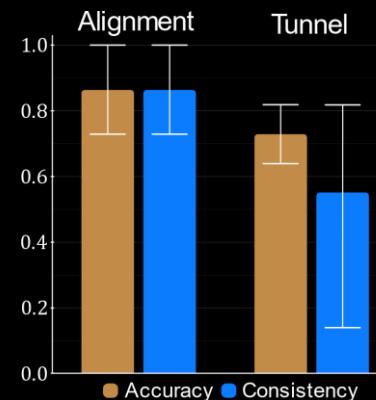
Silhouette (4)



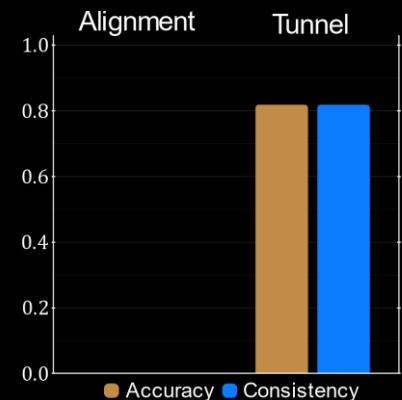
Depth (4)



Stability (2)



High-level (1)



[SLF\*11] Secord A. et al. – Perceptual Models of Viewpoint Preference – ACM TOG – 2011

[BFS\*18] Bonaventura X., et al. – A Survey of Viewpoint Selection Methods for Polygonal Models – Entropy – 2020

# Conclusion

## Alignment

- Surface metrics should be used: perfect results + cheap to compute

## Tunnel

- Depth entropy [MKS+21] has the best trade-off between computation time and efficiency ( $\approx 80\%$ )

No metric can find both configurations...

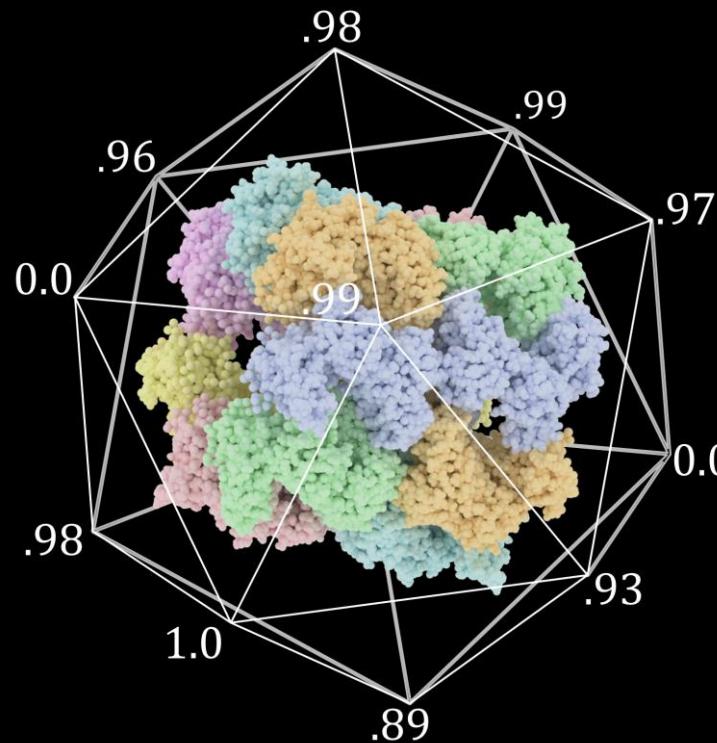
## Perspectives:

- Design new metrics (or combine existing ones) to improve the process and/or find other important features

# Molecular tour creation

Creation of an informative and visually pleasing tour of a molecule:

- Exploiting our viewpoint selection study
- Respecting some animation principles [Las87, SSBS07]



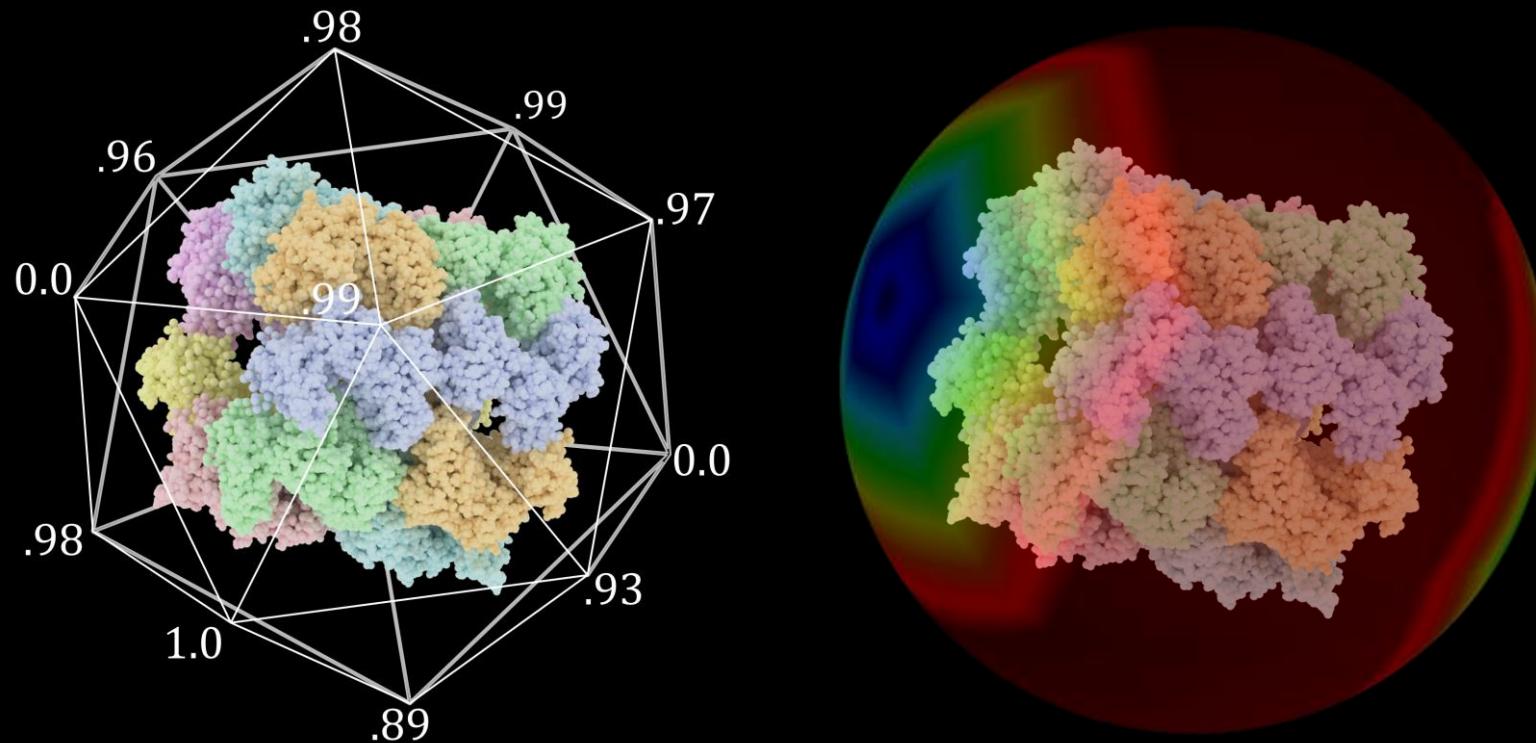
[Las87] Lasseter J. – Principles of traditional animation applied to 3D computer animation – Computer Graphics and Interactive Techniques – 1987

[SSBS07] Saleem W. et al. – On computing best fly – Spring Conference on Computer Graphics – 2007

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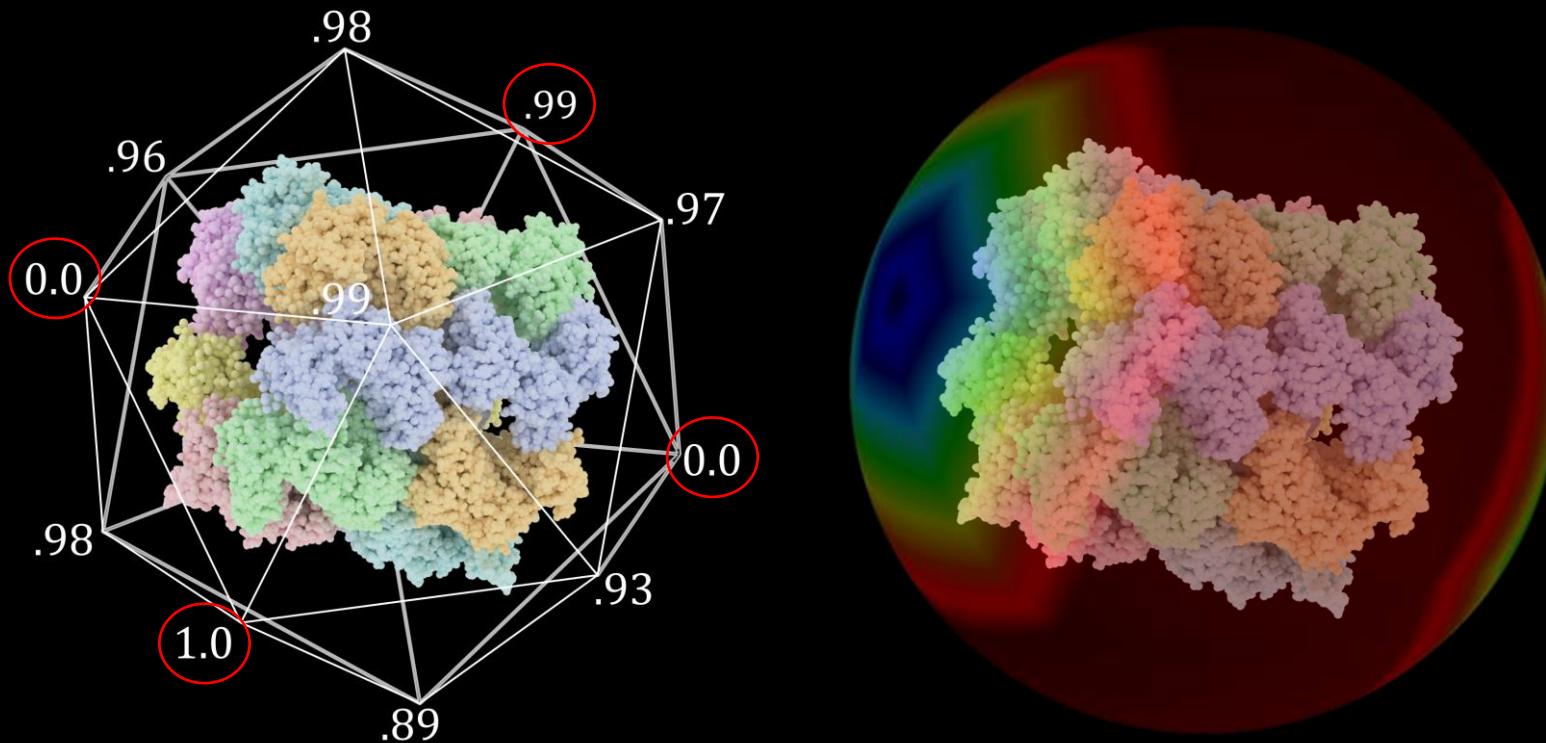
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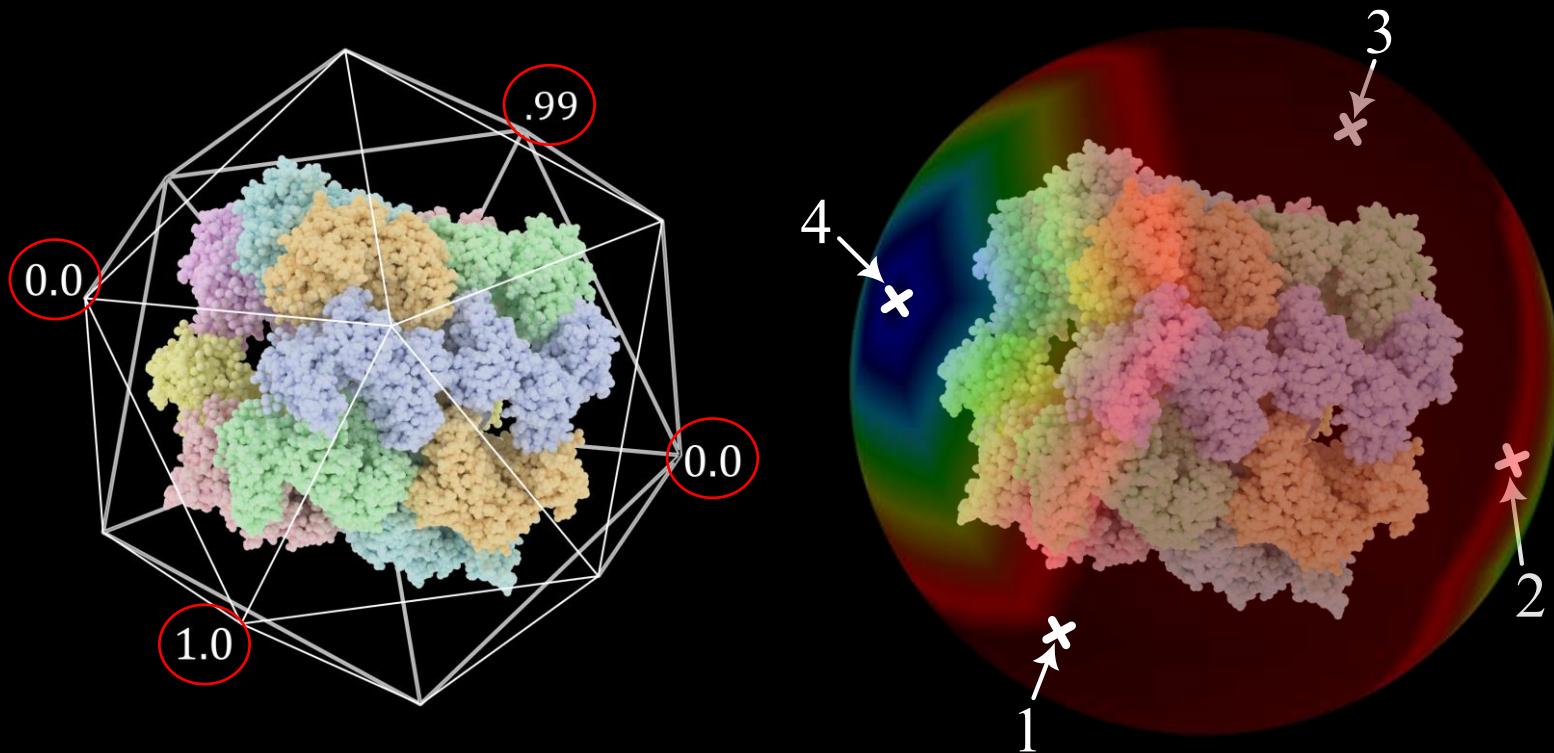
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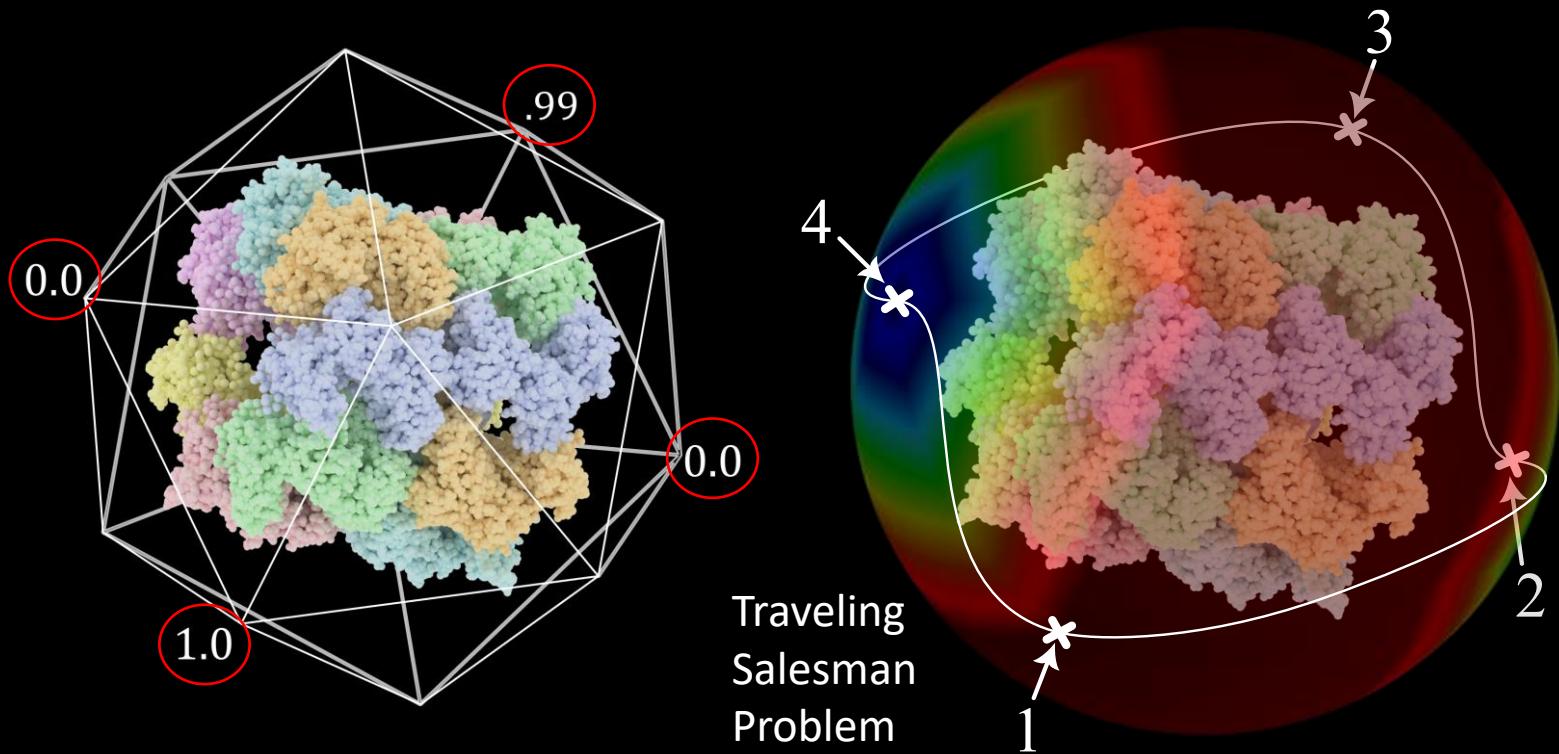
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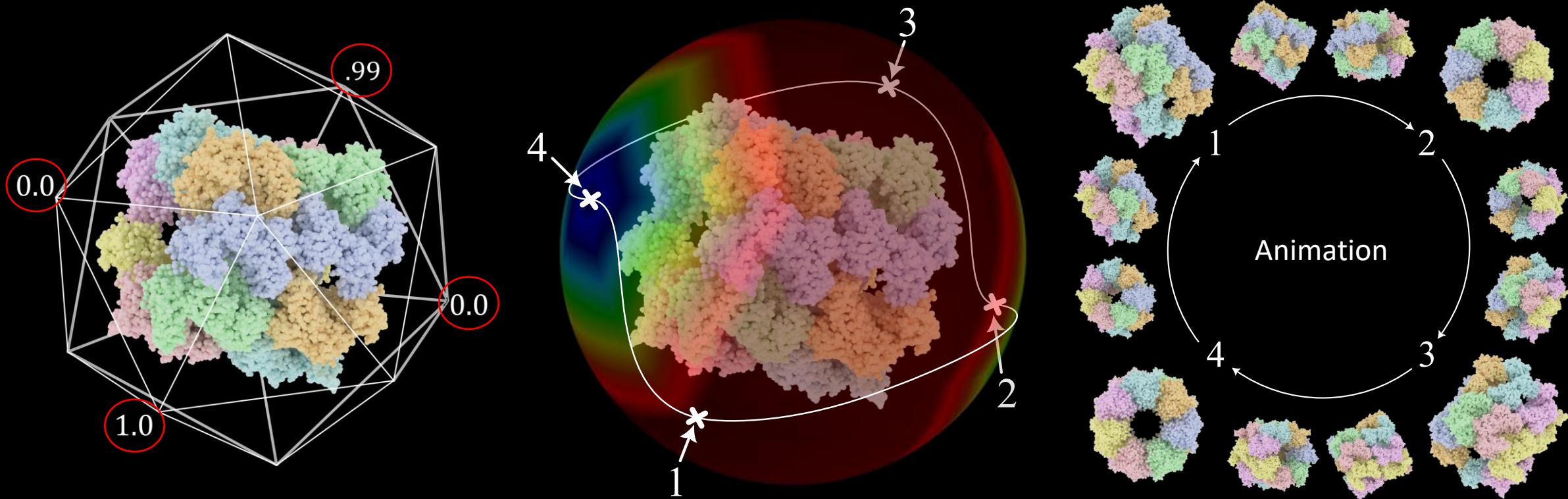
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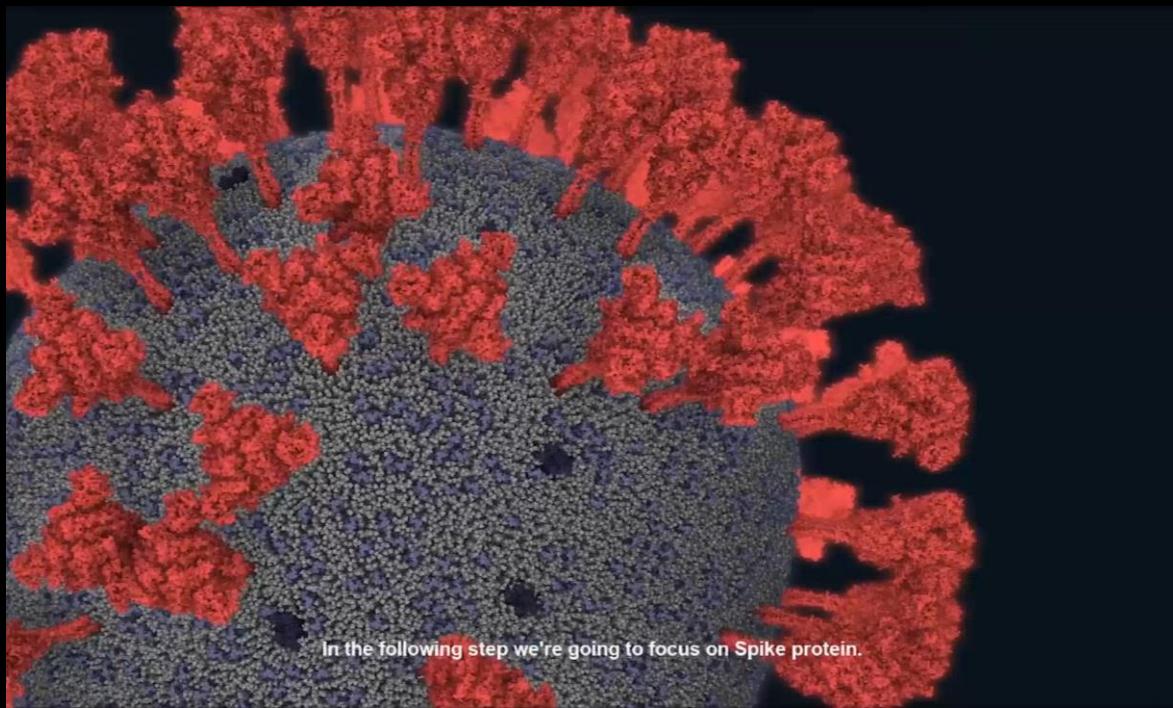
- Camera trajectory
- Pathfinding

# Related works

Only two related works (at our knowledge)

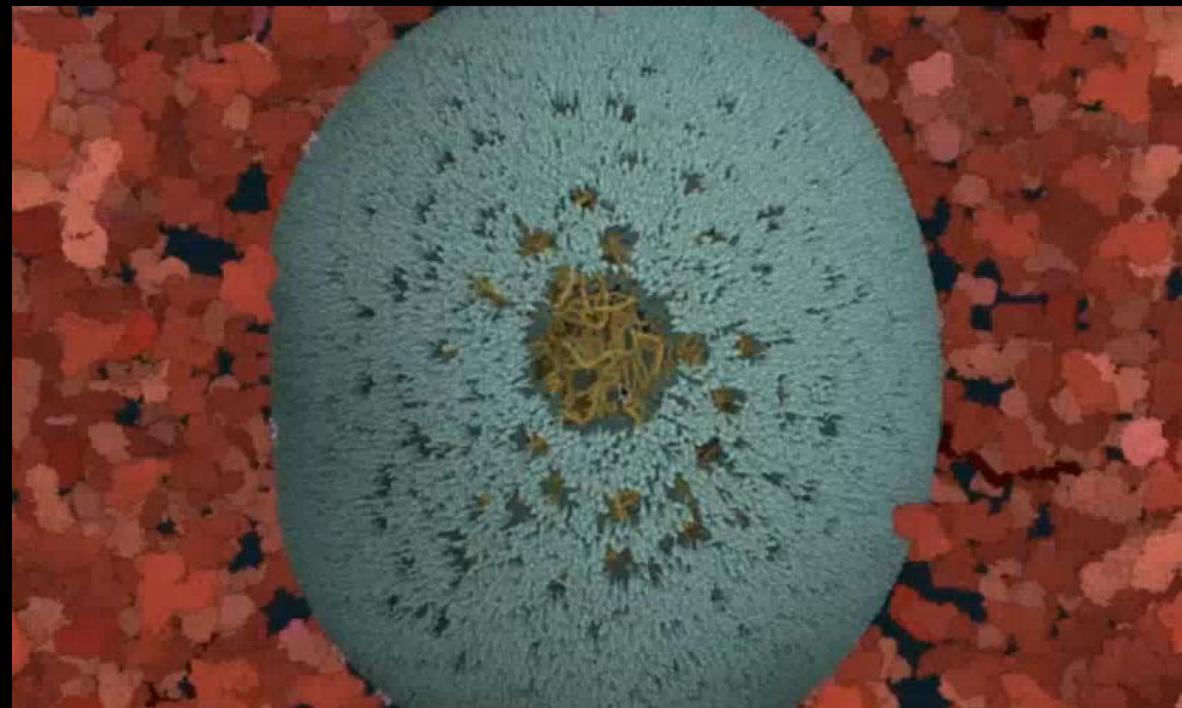
## Moleculetary [KSM\*21]

- Camera movement can be brutal



## Nanotilus [ASL\*21]

- Camera jerky + elements appear/disappear



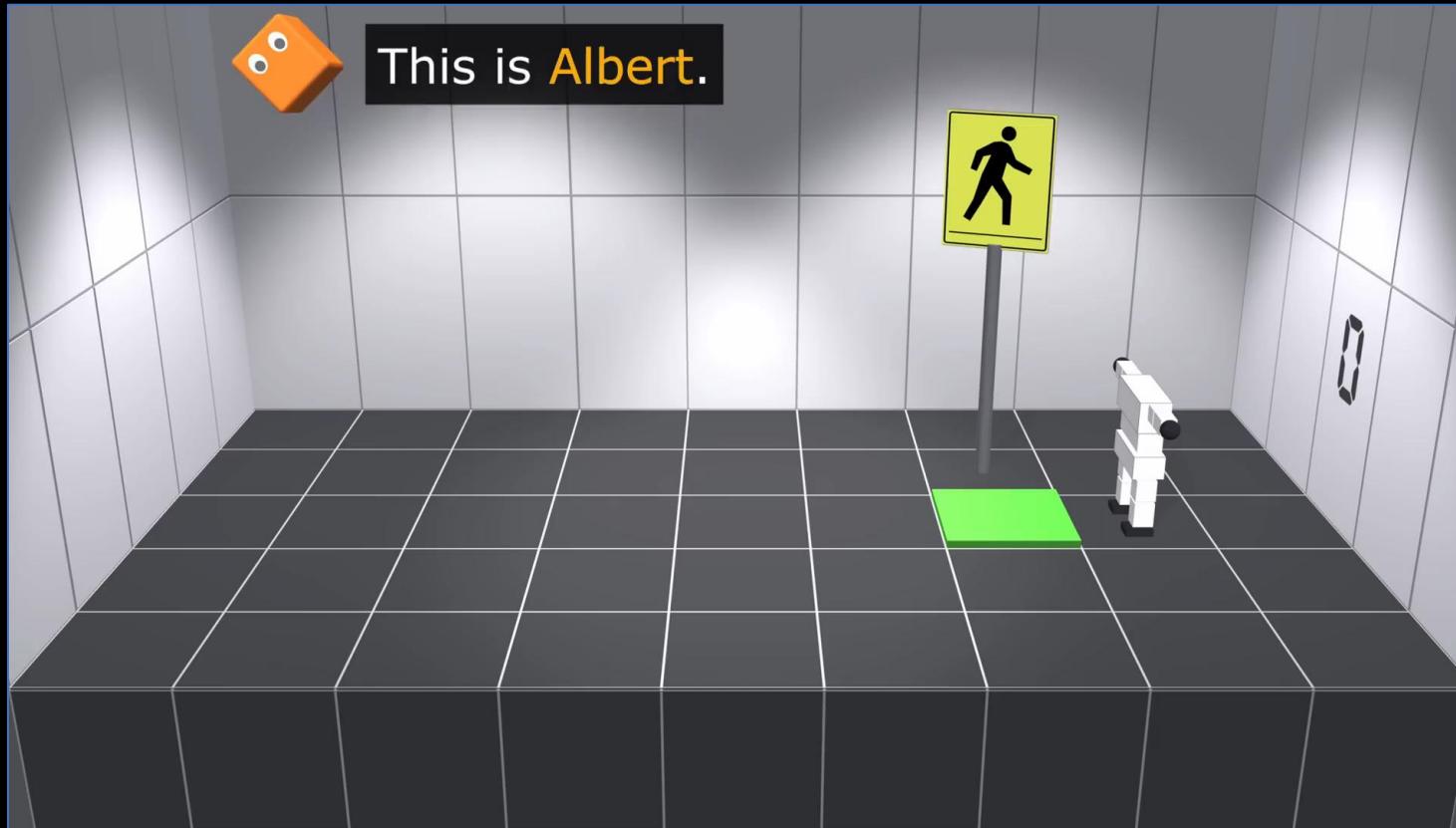
[KSM\*21] Kouřil D. – [Moleculetary: Scalable Narrated Documentaries Using Molecular Visualization](#) – IEEE TVCG – 2021

[ASL\*21] Alharbi R. et al. – [Nanotilus: Generator of Immersive Guided-Tours in Crowded 3D Environments](#) – IEEE TVCG – 2021

# (Very) early work !

Finding good camera trajectory between two points of interest

- Study related works for other things than molecules (*e.g.* drones)
- Idea: use Reinforcement Learning (RL)



AI Learns to Walk (deep reinforcement learning) – AI Warehouse : [https://youtu.be/L\\_4BPjLBF4E](https://youtu.be/L_4BPjLBF4E):

# What do we do in Limoges?

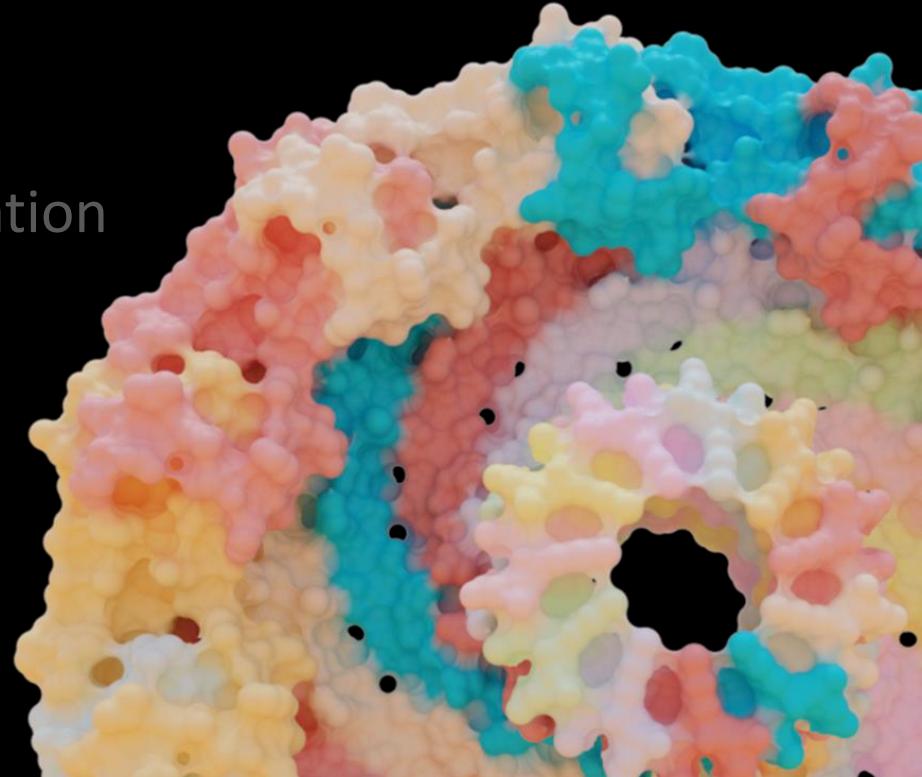
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Computer-aided generation of molecular simulation illustration

UDock2: Protein-protein docking



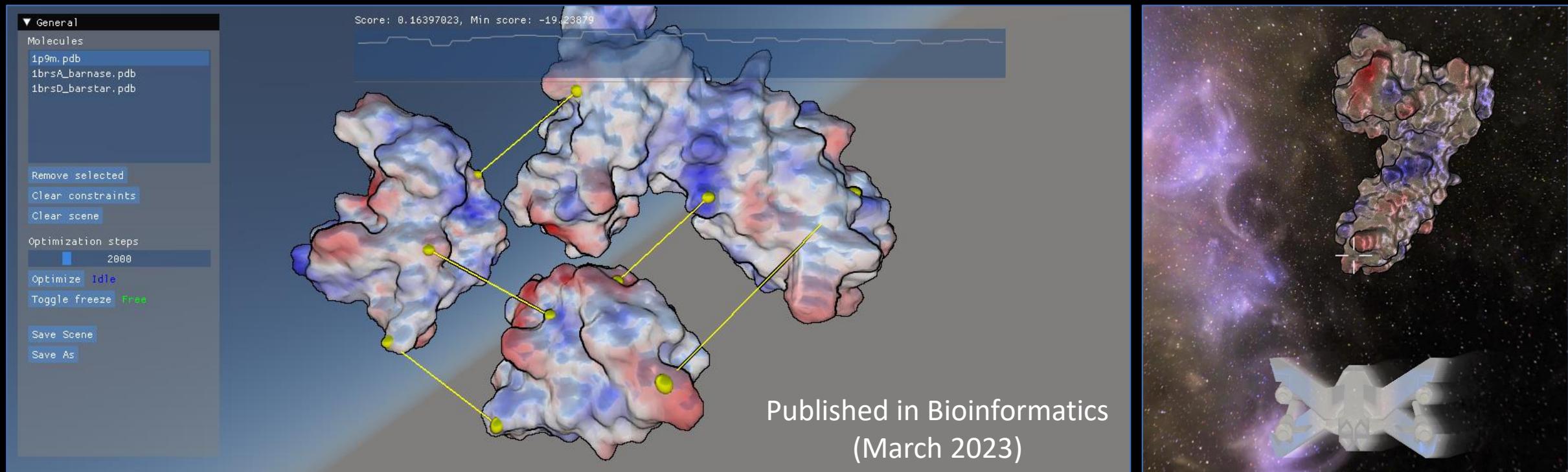
# UDock2

New version of UDock [GTM\*14] (collaborative work)

Interactive multibody docking with real-time energy calculation:

- Simple interface, intuitive usage

Gaming mode! Spaceship drivable with Xbox gamepad (for educational purposes and fun!)



[GTM\*14] Levieux G. et al. – Udock, the Interactive Docking Entertainment System – Faraday Discussions 168 – 2014

# THAT'S ALL FOLKS!

## Acknowledgments

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