EG23

SIC Saarland Informatics Campus

Automatic molecular tour creation: a study

Vincent Larroque[1], Maxime Maria[1], Stéphane Mérillou[1], Matthieu Montes[2]

[1]: Laboratoire XLIM, UMR CNRS 7252, Université de Limoges, France

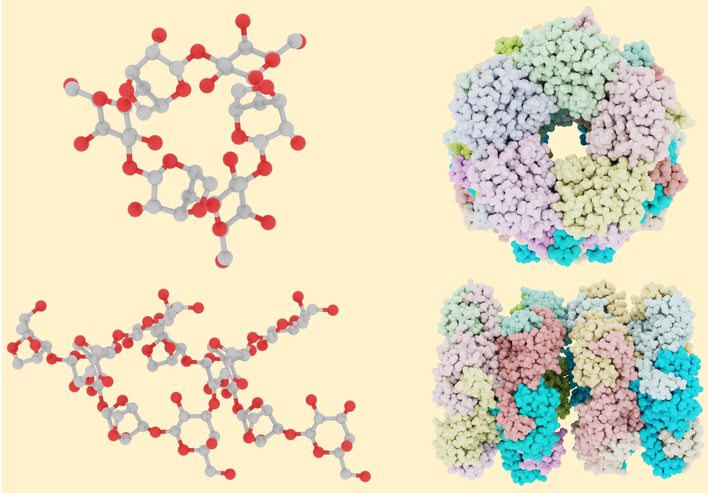
[2]: GBCM - Laboratoire Génomique, Bioinformatique et Chimie Moléculaire, EA7528, Conservatoire National des Arts et Métiers, Hésam Université, France

PROBLEM

- Computer simulations are essential for progress in drug design. For example, they allow rapid selection of potential drug candidates, according to their inhibitory effect on the target.
- Biochemists all over the world use molecular visualization software to explore molecular systems with millions of atoms in real-time.
- Molecules can be represented in various ways as described in Kozlíková *et al.* **[KKF*17]** overview of molecular visualization and must be considered when looking for interesting features.
- The geometric complexity of molecules makes exploration difficult, even for experts: we aim to provide a tool that will help the preliminary study of molecules by automatically creating a tour of the interesting viewpoints around it.

RELATED WORK

- Viewpoint selection for molecular visualization has been discussed in three specific papers:
  - Vázquez *et al.* **[VFSL06]** proposed an information theory-based method to select viewpoints of molecules.
  - Doulamis *et al.* **[DCMP10]** used input from domain experts to train a non-linear classifier to search for interesting viewpoints.
  - Heinrich *et al.* **[HVH*16]** expended **[VFSL06]** for another *molecular* representation and provided a study about viewpoint preferences.
- Vázquez and Heinrich defined two types of good viewpoints:
  - A viewpoint showing a lot of atoms and bonds, exposing most of the molecule (*figure 1*, *down*).
  - A viewpoint showing a geometrical configuration of the molecule (*figure 1*, *up*).
- Due to limited research specific to molecular visualization, our work consisted in finding and adapting general methods based on the surveys of Secord **[SFL*11]** and Bonaventura **[BFS*18]**.



Alignement **[VFSL06]** Tunnel **[HVH*16]**

Figure 1: Examples of molecular configurations (up) and another view of the same molecule (down).

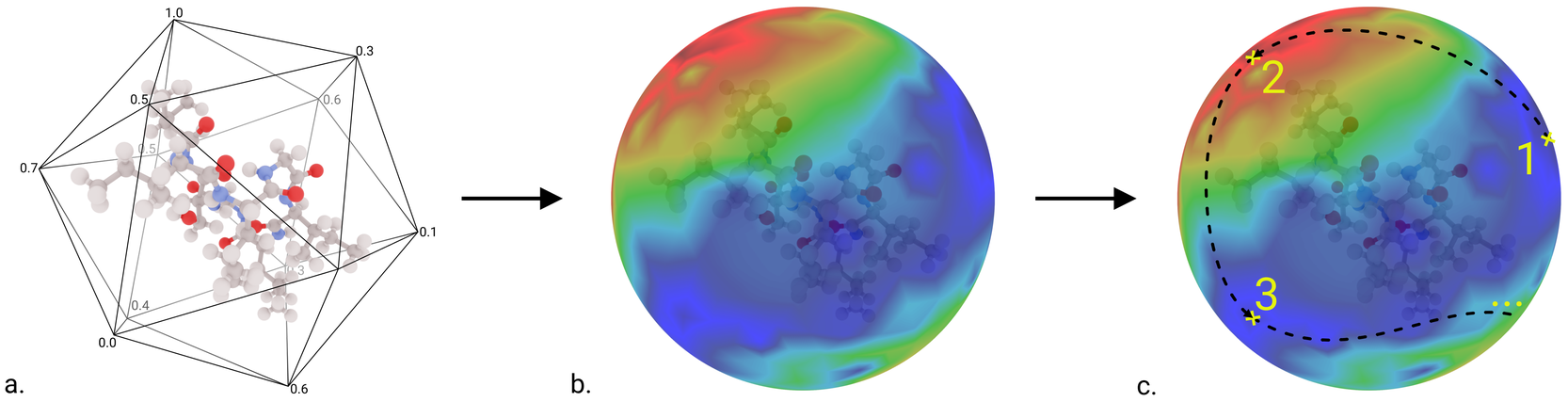
CONCLUSION

Our preliminary study exposes that our tool can generate molecular tours of interesting points of view around the molecule but cannot find specific geometrical configurations when requested. A larger study could provide more insight into our tool's true capabilities, but it is certain that new metrics specific to molecular visualization could provide benefits.

METHODOLOGY

The goal is to find the best viewpoints around a molecule: we must, at first, select the candidate viewpoints around it. To do so, we use the recursive discretization of an icosahedron, as shown in *figure 2.a*, to select regularly spaced points around the molecule.
The camera is placed on each of these points, looking at the molecule center, to compute an image. This image will then be analyzed by several metrics to compute a score based on its various visible properties. Finally, this score allows us to choose the best viewpoints, which have either the lowest or highest scores. Metrics are defined as $VQ(v) = F_m(v)$ where $VQ(v)$ is the quality score of a viewpoint v computed with the $F_m(v)$ metric function.

To build a molecular tour we use the projection of the icosahedron vertices containing the scores on an image to create a heatmap. This heatmap can be projected back onto a sphere to create the viewpoint sphere (*figure 2.b*) or to get the score for any point on it.
Researchers can visualize zones of interest using the viewpoint sphere itself, which are represented in blue (*low score*) and red (*high score*).
The molecular tour is created by filtering the extrema of the icosahedron giving us a list of points. The camera will be moving between each point using a Catmull-Rom spline, revealing interesting viewpoints along the way (*figure 2.c*).



a. b. c.

Figure 2: Pipeline of the molecular tour creation. (*a*) the icosahedron used to select viewpoints. (*b*) the corresponding viewpoint sphere. (*c*) the created molecular tour path.

RESULTS

We conducted a preliminary study with 10 molecules on the ability of metrics to detect a geometric configuration: the *"tunnel"*. Our results have shown that the molecule tour is able, for most measures, to show both a viewpoint exposing most of the molecule and a "tunnel" exposing viewpoint. *Figure 3.b* shows the resulting best viewpoint for a molecule. The metric used was the viewpoint entropy **[VFSL06]** with an icosahedron of 642 vertices. *Figures 3.b-1* and *3.b-3*, of low scores, are exposing the geometric configuration *"tunnel"* while the high scores in *figures 3.b-2* and *3.b-4* are viewpoints exposing most atoms of the molecule.

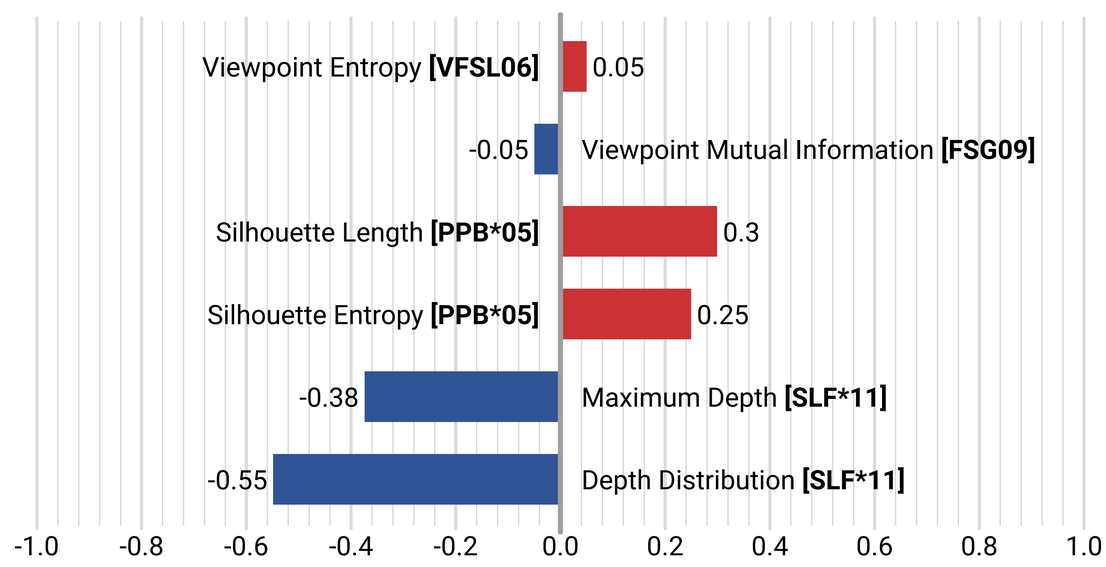


Figure 4: Precision of some viewpoint quality metrics.

Our study also showed that most metrics are unreliable: *figure 4* features a plot of the precision of some measures. The precision is calculated as the ability of a measure to reliably detect the *"tunnel"* geometrical configuration either on its highest (*red*) or lowest score (*blue*) or not at all. Precision goes from reliable (*±1*) to unreliable or unable to detect the feature at all (*0*).

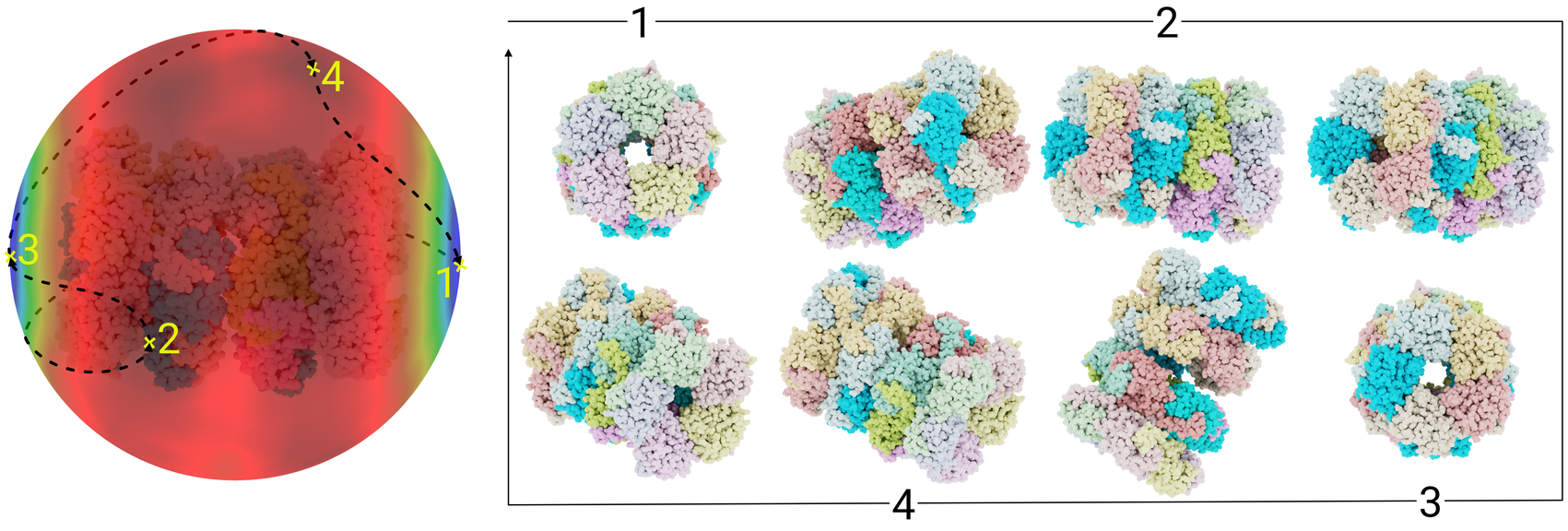


Figure 3: Result of the molecular tour with key viewpoints (*1, 2, 3 and 4*) and their intermediary viewpoints.

REFERENCES

[BFS*18] BONAVENTURA X., FEIXAS M., SBERT M., CHUANG L., ALLRAVEN C.: **A Survey of Viewpoint Selection Methods for Polygonal Models.** *Entropy 20*, 5 (2018), 370.

[DCMP10] DOULAMIS N., CHRONIS E., MIAOULIS G., PLEMENOS D.: **Personalized View Selection of 3D Molecular Proteins. In Intelligent Computer Graphics 2010.** *Springer Berlin Heidelberg*, 2010, pp. 211–227.

[KKF*17] KOZLÍKOVÁ B., KRONE M., FALK M., LINDOW N., BAADEN M., BAUM D., VIOLA I., PARULEK J., HEGE H.-C.: **Visualization of Biomolecular Structures: State of the Art Revisited.** *Computer Graphics Forum 36*, 8 (2017), 178–204.

[SLF*11] SECORD A., LU J., FINKELSTEIN A., SINGH M., NEALEN A.: **Perceptual Models of Viewpoint Preference.** *ACM Trans. Graph. 30*, 5 (Oct. 2011), 1–12.

[VFSL06] VÁZQUEZ P.-P., FEIXAS M., SBERT M., LLOBET A.: **Realtime automatic selection of good molecular views.** *Computers & Graphics 30*, 1 (2006), 98–110.

[PPB*05] POLONSKY O., PATANÉ G., BIASOTTI S., GOTSMAN C., PAGNUOLO M.: **What's in an image?** *The Visual Computer 21*, 8 (Sept. 2005), 840–847.

[FSG09] FEIXAS M., SBERT M., GONZÁLEZ F.: **A Unified Information-Theoretic Framework for Viewpoint Selection and Mesh Saliency.** *ACM Trans. Appl. Percept. 6*, 1 (Feb. 2009).

[HVH*16] HEINRICH J., VUONG J., HAMMANG C. J., WU A., RITTENBRUCH M., HOGAN J., BRERETON M., O'DONOGHUE S. I.: **Evaluating Viewpoint Entropy for Ribbon Representation of Protein Structure.** *Computer Graphics Forum 35*, 3 (June 2016), 181–190.

cnrs Université de Limoges

INSTITUT DE RECHERCHE xlim le cnam gbcm