Biomolecule Visualization

Subjects: Biochemistry & Molecular Biology

Contributor: Hui Li , Xinru Wei

The structural characteristics of biomolecules are a major focus in the field of structural biology. Molecular visualization plays a crucial role in displaying structural information in an intuitive manner, aiding in the understanding of molecular properties.

molecular visualization
computer graphics
representation models
level of detail
augmented reality

1. Representation Models

Biological molecules exhibit high complexity and diversity, and are composed of atoms connected through specific chemical bonds and interactions. To express their three-dimensional configuration and spatial arrangement, different representation models can be used, as shown in **Figure 1**. This section categorizes representation models into skeletal models, cartoon models, and surface models.

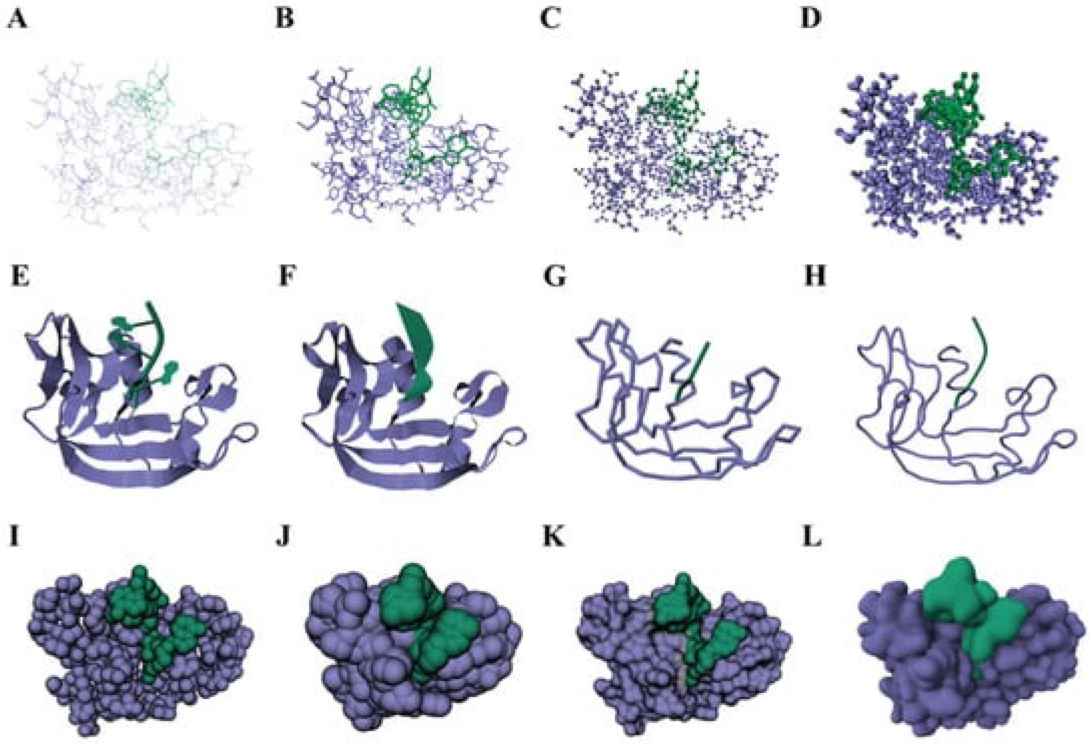

Figure 1. The different representation models of Ribonuclease (PDB ID: 1M07) including: (**A**) lines model, (**B**) stick model, (**C**) ball-and-stick model, (**D**) HyperBall model, (**E**) cartoon model, (**F**) ribbon model, (**G**) backbone model,

(**H**) trace model, (**I**) vdW surface (space-filling model), (**J**) SAS surface, (**K**) SES surface, and (**L**) Gaussian surface. UnityMol (http://www.baaden.ibpc.fr/umol/ (accessed on 15 October 2023)) [1], MegaMol (https://megamol.org/ (accessed on 15 October 2023)) [2], and the integrated molecular viewer in RCSB PDB (https://www.rcsb.org/3d-view/ (accessed on 15 October 2023)) are used for visualization. Different colors represent separate chains within a molecule.

Skeletal models describe the backbone structure of molecules, including atoms, chemical bonds, and their spatial topology. They use simple geometric shapes like line segments, spheres, cylinders, and polyhedra to represent the model's structure. Skeletal models are one of the simplest and oldest representation methods. Most molecular visualization software currently implements skeletal models, such as lines models, stick models, ball-and-stick models, and space-filling models.

The lines model (**Figure 1**A) is a representation method using lines to connect atoms and emphasizes the basic features and geometric relationships within the structure. The stick model (**Figure 1**B) is similar to the lines model, but it uses sticks to connect atoms. Ball-and-stick models (**Figure 1**C) and space-filling models (**Figure 1**I) use spheres to represent atoms, with each sphere's radius typically being proportional to the corresponding atomic radius. This facilitates an understanding of the relative positions and structural relationships of atoms in the molecule. Space-filling models can also represent the spatial occupancy of atoms through the size and position of the spheres, revealing gaps and channels in the molecular structure. In addition to these common representation models, Chavent et al. [3] introduced a new method called HyperBall (**Figure 1**D), which uses hyperboloids to connect atoms represented in the form of spheres. HyperBall achieves a higher rendering efficiency and quality than triangle meshes inspired by GPU ray casting techniques.

Cartoon models integrate the representation of atoms and chemical bonds into ribbon-like or tubular structures, highlighting overall structural features. They are commonly used for proteins. Richardson [4] first proposed using ribbons and arrows to represent protein secondary structure, and Carson et al. [5] were the first to implement it programmatically. Cartoon representations of proteins are integrated into almost all molecular visualization software. Classic cartoon models (**Figure 1**E) and ribbon models (**Figure 1**F) can highlight protein secondary structure features and describe protein folding behavior. Backbone models (**Figure 1**G) show the folding of the polypeptide chain by creating artificial "backbone" bonds between alpha carbons.Trace models (**Figure 1**H) use a smooth curve to display the backbone. The hermite spline curve passes through the mid-points between alpha carbon atoms [6]. They are commonly used to emphasize the overall structure and topological relationships of proteins. Researchers have focused on improving the visualization performance of cartoon models through mesh refinement techniques and GPU acceleration techniques [7]. Recently, Borzov [8] proposed a new method using signed distance fields and sphere tracing techniques for cartoon protein representation, explaining the underlying mathematical characteristics and comparing them with existing mesh refinement methods. Ozvoldik et al. [9] successfully introduced LOD techniques into grid-based molecular model visualization, achieving cartoon model renderings for larger-scale protein data.

Surface models are obtained by computing the surfaces connecting the molecule to the surrounding environment, helping us to understand the interactions between molecules resulting from various chemical bonds. The most basic surface model is the Van der Waals Surface (vdW) (**Figure 1**I) [10], which is the outer surface formed by the combination of all atomic spheres in the space-filling model. A surface model shows the volume occupied by the molecule, with the radius of the atomic spheres being proportional to the Van der Waals radius. Lee and Richards created the Solvent Accessible Surface (SAS) (**Figure 1**J) [11], defined as the surface formed by the rolling motion of solvent molecule probes on the vdW surface. It displays all regions from which solvent molecules can enter the molecule but cannot accurately represent the volume of the molecule. Richards and Greer further researched and defined the Solvent Excluded Surface (SES) (**Figure 1**K) [10][12] as the surface formed by the probes' contact points with the molecule, which accurately reflects the molecular volume and expresses the accessibility of the molecule, helping to describe the interactions between the molecule and its surrounding environment.

Blinn [13] proposed the Gaussian convolution surface (**Figure 1**L) implicit surface modeling algorithm, commonly used in electron density analysis to simulate the electron density map of molecular structures. From a mathematical perspective, the SES surface is the first smooth molecular surface and has attracted extensive attention and research. Connolly [14] developed a program to calculate and display the SES surface. Chavent et al. [15] used a GPU to compute a completely continuous molecular skin surface, pioneering the application of GPU in molecular surface calculation. Recent research in this field focuses on fast construction algorithms for SES surfaces, utilizing high-performance GPU acceleration or general-purpose CPU acceleration without hardware limitations. Examples include the GPU algorithms by Hermosilla et al. [16], Martinez et al. [17], Schäfer et al. [18], Alhazzazi et al. [19], and the CPU algorithm by Rau et al. [20].

Martinez et al. [17] completed an open-source implementation of the work carried out by Hermosilla et al. [16] and developed the QuickSES library to integrate it into molecular viewers, providing a standalone program that reads PDB files and outputs a complete SES mesh as a Wavefront OBJ file. In addition, new methods for constructing molecular surfaces have emerged. Hermosilla [21] introduced the use of transparency to improve the visual perception of molecular surfaces and proposed a fast method for calculating and implementing rendering of transparent and translucent materials. Bruckner [22] proposed a dynamic visibility-driven molecular surface visualization method based on Gaussian models, allowing for the dynamic high-quality surface visualization of molecules composed of millions of atoms. Wei et al. [23] introduced a machine learning algorithm that can predict classical SES surfaces on proteins and complex structures, achieving a higher computational efficiency and over 95% accuracy compared to CPUs.

2. Rendering Technology

The field of molecular visualization utilizes various rendering techniques to enhance the visual representation of molecules. These techniques include ray tracing, ambient occlusion, illustrative rendering, non-photorealistic rendering, and color mapping. **Figure 2** showcases the various rendering effects of cartoon models and molecular surfaces.

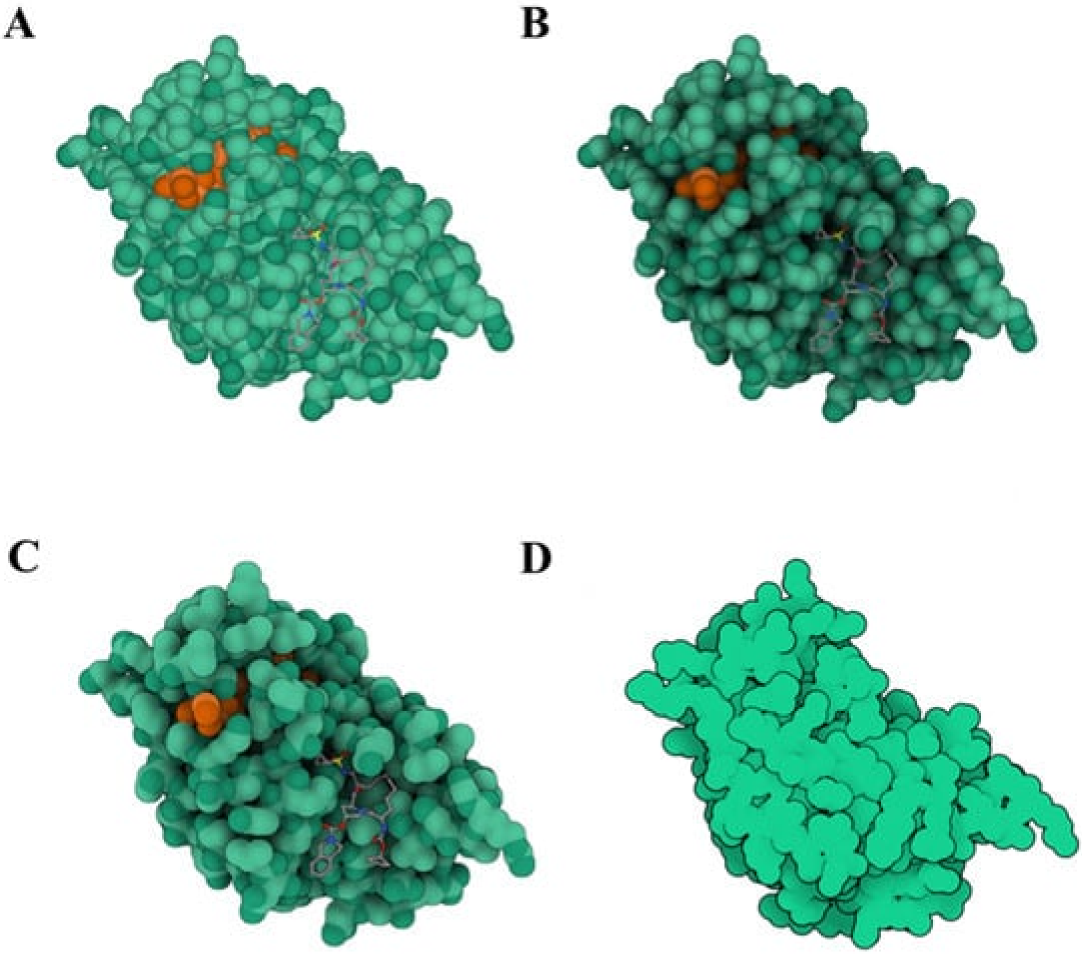

Figure 2. The protease inhibitor (PDB ID: 4KTC) can be rendered in four different ways: (**A**) local illumination rendering, (**B**) ambient occlusion rendering, (**C**) illustrative rendering, and (**D**) PDB-101 style illustration. Molstar [24] and Illustrate [25] are used for visualization. Different colors represent separate chains within a molecule.

Initially, macromolecule shadow surfaces were created using rasterization rendering [26]. However, ray tracing techniques have gradually gained popularity in molecular visualization. BALLView [27], one of the earliest molecular visualization tools, combines real-time ray tracing rendering, which has become a focus of research into visualization rendering methods. Achieving real-time performance in rendering requires algorithm parallelism and designing acceleration structures. Stone [28] summarizes interactive ray tracing and compatible rendering techniques applicable to molecular visualization and provides example codes.

To improve rendering quality, lighting models can be used to simulate reflection, refraction, and other real-world object phenomena. The Blinn–Phong local lighting model proposed by Phong [29] and Blinn [30] significantly enhances the quality and speed of real-time rendering. However, this model cannot express shadows cast by atoms onto each other in molecular visualization. To address this, ambient occlusion (AO) techniques have been proposed by Miller [31] and Zhukov [32]. AO techniques approximate global lighting models by collecting diffuse reflection information from around objects. They capture scene details, enhance stereo perception, and improve realism. For example, Tarini et al. [33] combined ambient occlusion and edge highlighting using a GPU-accelerated algorithm to enhance the real-time visualization of molecular space-filling models. Matthews et al. [34] proposed a per-pixel ambient occlusion algorithm suitable for visualizing the dynamic scenes of proteins. Hermosilla et al. [35] proposed a universal global lighting model for various molecular models. Zerari et al. [36] combined SSAO (screen space ambient occlusion) technology with multiple importance sampling techniques to accelerate real-time rendering. Rau et al. [20] utilized CPU-based ray tracing technology to interactively visualize SES (solvent-excluded surface) surfaces, achieving high-quality rendering by combining the techniques into AOOM (Ambient Occlusion Opacity Mapping).

Illustrative rendering and non-photorealistic rendering techniques create artistic effects which are different to traditional realistic rendering, imitating hand-drawn, cartoon, sketch, and other art styles. Lawonn et al. [37] reviewed illustrative rendering techniques and their practical applications, not limiting them to molecular structure visualization. Koch et al. [38] proposed a molecular illustrative representation method utilizing screen space lighting algorithms, aiding in perceiving the hierarchical structure of multi-scale models. Liang et al. [39] presented a GPU-based boundary ellipsoid abstraction representation that emphasizes the surface details of molecules using contours, making molecular visualization visually appealing and informative. Illustrative rendering and non-photorealistic rendering simplify complexity and highlight key features, making them suitable for education and communication. The education website PDB-101 (https://pdb101.rcsb.org/ (accessed on 15 October 2023)) maintained by RCSB PDB uses 2D illustrations of molecular models generated directly by Illustrate [25].

Color is commonly used in molecular visualization to visually differentiate components. Waldin et al. [40][41] proposed a dynamic multiscale color mapping technique that adaptively adjusts the color scheme based on the current view and scale, ensuring the optimal representation of structural information at any given scale. CellVIEW [42] and YASARA View [43] combine LOD technology to realize the automatic color conversion of complex biomolecules. **Figure 3** showcases an application example of color mapping technology in YASARA View. However, color selection in molecular visualization often depends on cultural factors or personal preference. Inconsistent semantic color spaces can reduce the overall interpretability and effectiveness of molecular visualization. Garrison et al. [44] provide color palette samples for industrial and research sectors and propose considerations for developing best practices in color palettes.

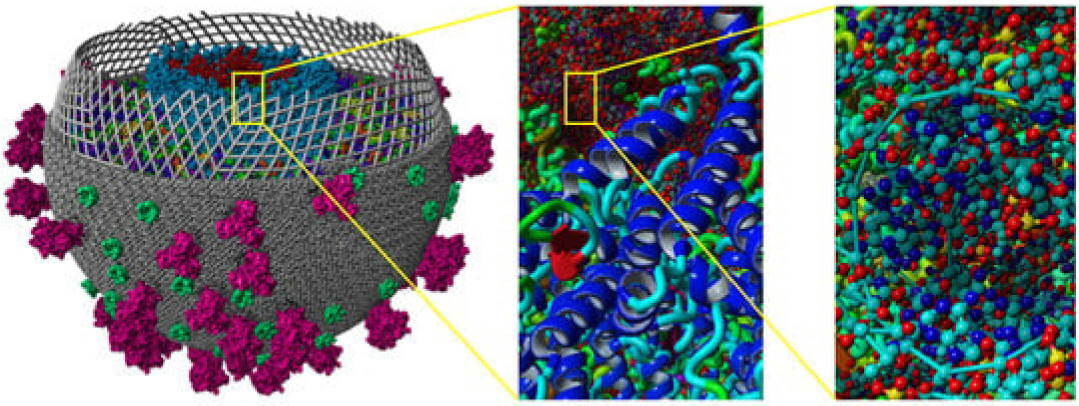

Figure 3. YASARA View (http://www.yasara.org/ (accessed on 15 October 2023)) [43] is used to visualize HIV at a mesoscopic level. The LOD technique is used with the appropriate level of detail. The color scheme is adjusted

adaptively.

In practical applications of molecular visualization, a combination of various rendering techniques is often used to aid in the analysis of complex structures. MegaMol [2] and Molstar [24] integrate advanced lighting algorithms for the efficient rendering of molecular data, with Molstar being capable of online rendering using multiple algorithms.

3. LOD Technology

In complex molecular visualization scenarios, when the camera is far from the atoms or when the atoms are scaled down to a volume smaller than one pixel, the projection on the screen becomes very small, resulting in limited visually recognizable information. To maintain visual effectiveness while reducing model complexity and speeding up rendering, the technique of Level of Detail (LOD) can be used. LOD involves using simplified models for distant observation or low zoom levels, reducing the number of vertices and faces to improve rendering performance. For close observation or high zoom levels, more detailed models are used to maintain detail and realism.

Guo et al. [45] proposed an LOD representation method for visualizing atomic structures in biology. They used an approximation error metric to evaluate the error of sphere simplification, achieving high-precision rendering and adaptive LOD selection based on the view. Liang et al. [39] utilized LOD techniques to reduce the number of primitives for rendering molecular surfaces, achieving a hierarchical abstraction representation of large molecules and distance-based LOD selection to ensure symmetrical structures have the same representation. Ozvoldik et al. [9] proposed a mesh-based LOD algorithm for LOD rendering of commonly used models such as ball-and-stick models and cartoon models for particularly large biomolecules.

LOD techniques are effective methods for achieving multi-scale visualization [46] and mid-scale visualization [43], especially when dealing with complex datasets or scenes that require smooth transitions and detail switching between different levels. CellVIEW [42] utilizes the Unity3D game engine to interactively visualize large molecular datasets, automatically selecting appropriate colors and detail levels using innovative LOD techniques to achieve seamless visual transitions between different abstraction levels. Goodsell et al. [43] connect the nanometer scale of molecules with the micrometer scale of cells through mid-scale modeling and visualization to simulate the molecular structure of living cells. LOD techniques are used to select appropriate detail levels and keep computational demands within achievable limits, providing sufficient detail to support recognition and understanding, as shown in **Figure 3**.

Additionally, LOD techniques can also help achieve high frame rate rendering on immersive visualization devices [47]. Goddard et al. [48] used LOD techniques to render complex molecular scenes at high frame rates in virtual reality environments.

4. Positional Uncertainty Visualization Technology

Biomolecules exhibit dynamic and flexible behavior, which introduces positional uncertainty. Additionally, the process of collecting and processing data introduces uncertainties. These uncertainties can arise from experimental data due to resolution limitations, simulated data generated by simulation algorithms, and visualized data obtained through analysis algorithms prior to visualization. It is crucial to accurately and honestly represent these uncertainties in visualizations.

The dynamics and flexibility of biomolecules can be studied using molecular dynamics simulations. However, these simulations require extensive computing resources and high frame rate rendering algorithms. In current research, processed static structures have been primarily used to visualize the uncertainty in atomic positions, rather than dynamic images or videos. Commonly used representations for depicting this uncertainty in atomic positions in proteins include sausage-like representations, such as the “sausage” view in MolMol [49] and the “putty” representation in PyMOL [50]. These representations allow for the drawing of tubular splines with variable radii, where larger radii indicate greater uncertainty in atomic positions. The color change in the sausage plot can be determined by the B factor, which is a parameter used in X-ray diffraction experiments to describe the position uncertainty caused by thermal vibrations of atoms in a crystal. Higher B-factors in sausage plots generally correspond to larger uncertainties and are represented by cooler tones. These color changes can help observers intuitively understand the uncertainty of atoms at different positions. Additionally, the uncertainty in the molecule can be represented using a molecular surface colored according to the B-factor, as shown in **Figure 4**.

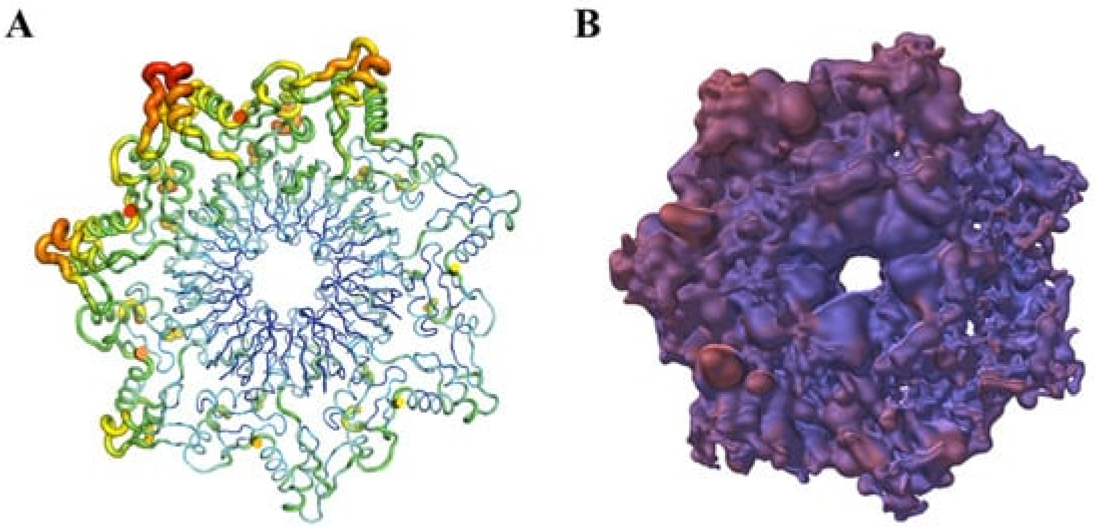

Figure 4. The uncertainty visualization of the bacterial protein (PDB ID: 1M5Q) using PyMol [50] and UnityMol [1]. (**A**) Sausage representation, (**B**) molecular surface.

Sterzik et al. [51][52] mapped uncertainty introduced during data acquisition and processing onto solvent-excluded surface (SES), van der Waals (vdW) surface, and cartoon models using stylized lines. Perception studies were conducted to determine the effectiveness of five line variables (roughness, jitter, grayscale, width, and blur) in distinguishing various uncertainty values in molecular representation models. The results indicated that width and grayscale achieved better results, although grayscale was more sensitive to color changes in the molecular representation models. Roughness and blur only applied to medium-high uncertainty differences, with roughness also requiring less dense lines. Jitter had the least effective outcome. Future work may focus on the combined application of line variables and stylized line generation algorithms, while considering interference with the perception of other characteristics. Schulz et al. [53] represented uncertainty by uniformly distorting the geometric structure of standard molecular representation models in all directions using periodic waveforms, where the uncertainty arose from inconsistencies in secondary structure assignments.

Discrete representation and possibility volume representation are alternative methods for visualizing the uncertainty in atomic positions [54]. Discrete representation treats atomic positions as independent points and uses transparency to express the probability of each position's existence. Although this approach provides highly detailed and accurate information, the resulting images may be overly complex and difficult to interpret. Possibility volume representation treats atomic positions as a three-dimensional grid in continuous space and colors the grid based on probability density functions. Maack et al. [55] used volume rendering and combined techniques such as transparency and B-factor coloring to visualize the uncertainty in atomic positions, providing a visual analytical framework for protein data with uncertainty. This uncertainty captures variations in atomic positions due to imprecise measurements or multi-model calculations.

5. Immersive Visualization Technology

Molecular immersive visualization utilizes Virtual Reality (VR) or Augmented Reality (AR) technologies to visualize molecular structures, enhancing the observer's intuitive perception of complex structures and spatial relationships.

VR technology places users in a completely virtual and immersive simulated environment, isolated from the real environment. Users typically wear specialized VR devices such as head-mounted displays, sensors, and headphones to experience the virtual environment. Kuťák et al. [56] provide a detailed overview of molecular immersive rendering using modern head-mounted platforms and list a range of available tools. Game sensors [57] and force feedback gloves [58] enable hand-controlled molecular virtual reality.

On the other hand, AR technology superimposes virtual elements onto the real world to expand users' perception of the real world. This can be achieved on mobile devices such as smartphones and tablets, for example, StereoChem [59] and Augment [60].

The development and reduction in the price of computer hardware, especially head-mounted displays, have led to the emergence of numerous molecular immersive visualization technologies and tools. One approach to developing these tools is integrating existing tools into immersive environments. For example, Dimmol is based on UnityMol [61], ChimeraX is based on Chimera [48], and CootVR is based on Coot [62]. To provide a smooth visual experience, molecular immersive visualization requires rendering technologies that support low latency and high frame rates.

References

1. Doutreligne, S.; Cragnolini, T.; Pasquali, S.; Derreumaux, P.; Baaden, M. UnityMol: Interactive scientific visualization for integrative biology. In Proceedings of the 2014 IEEE 4th Symposium on Large Data Analysis and Visualization (LDAV), Paris, France, 9–10 November 2014; pp. 109–110.
2. Grottel, S.; Krone, M.; Müller, C.; Reina, G.; Ertl, T. MegaMol—A prototyping framework for particle-based visualization. IEEE Trans. Vis. Comput. Graph. 2014, 21, 201–214.
3. Chavent, M.; Vanel, A.; Tek, A.; Levy, B.; Robert, S.; Raffin, B.; Baaden, M. GPU-accelerated atom and dynamic bond visualization using hyperballs: A unified algorithm for balls, sticks, and hyperboloids. J. Comput. Chem. 2011, 32, 2924–2935.
4. Richardson, J.S. The anatomy and taxonomy of protein structure. Adv. Protein Chem. 1981, 34, 167–339.
5. Carson, M.; Bugg, C.E. Algorithm for ribbon models of proteins. J. Mol. Graph. 1986, 4, 121–122.
6. Jmol: An Open-Source Java Viewer for Chemical Structures in 3D. Available online: http://www.jmol.org/ (accessed on 15 October 2023).
7. 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. Comput. Graph. Forum 2017, 36, 178–204.
8. Borzov, S. Use of Signed Distance Functions for the Definition of Protein Cartoon Representation. Master’s Thesis, Masarykova Univerzit, Brno, Czech Republic, 2021.
9. Ozvoldik, K.; Stockner, T.; Rammner, B.; Krieger, E. Assembly of biomolecular gigastructures and visualization with the vulkan graphics API. J. Chem. Inf. Model. 2021, 61, 5293–5303.
10. Richards, F.M. Areas, volumes, packing, and protein structure. Annu. Rev. Biophys. Bioeng. 1977, 6, 151–176.
11. Lee, B.; Richards, F.M. The interpretation of protein structures: Estimation of static accessibility. J. Mol. Biol. 1971, 55, 379–400.
12. Greer, J.; Bush, B.L. Macromolecular shape and surface maps by solvent exclusion. Proc. Natl. Acad. Sci. USA 1978, 75, 303–307.
13. Blinn, J.F. A generalization of algebraic surface drawing. ACM Trans. Graph. (TOG) 1982, 1, 235–256.
14. Connolly, M.L. Solvent-accessible surfaces of proteins and nucleic acids. Science 1983, 221, 709–713.
15. Chavent, M.; Levy, B.; Maigret, B. MetaMol: High-quality visualization of molecular skin surface. J. Mol. Graph. Model. 2008, 27, 209–216.

16. Hermosilla, P.; Krone, M.; Guallar, V.; Vázquez, P.P.; Vinacua, À.; Ropinski, T. Interactive gpu-based generation of solvent-excluded surfaces. Vis. Comput. 2017, 33, 869–881.
17. Martinez, X.; Krone, M.; Baaden, M. QuickSES: A library for fast computation of solvent excluded surfaces. In Proceedings of the MolVa: Workshop on Molecular Graphics and Visual Analysis of Molecular Data 2019, Porto, Portugal, 3 June 2019.
18. Schäfer, M.; Krone, M. A Massively Parallel CUDA Algorithm to Compute and Visualize the Solvent Excluded Surface for Dynamic Molecular Data. In Workshop on Molecular Graphics and Visual Analysis of Molecular Data; The Eurographics Association: Porto, Portugal, 2019.
19. Alhazzazi, M.; Hayward, S.; Laycock, S.D. GPU-Accelerated Generation of the Molecular Surface. In Proceedings of the Eurographics (Posters), Norrköping, Sweden, 25–29 May 2020; pp. 9–10.
20. Rau, T.; Zahn, S.; Krone, M.; Reina, G.; Ertl, T. Interactive CPU-based Ray Tracing of Solvent Excluded Surfaces. In Proceedings of the VCBM, Brno, Czech Republic, 4–6 September 2019; pp. 239–251.
21. Hermosilla Casajús, P.; Maisch, S.; Vázquez Alcocer, P.P.; Ropinski, T. Improving perception of molecular surface visualizations by incorporating translucency effects. In Proceedings of the VCBM 2018: Eurographics Workshop on Visual Computing for Biology and Medicine, Granada, Spain, 20–21 September 2018; pp. 185–195.
22. Bruckner, S. Dynamic Visibility-Driven Molecular Surfaces. Comput. Graph. Forum 2019, 38, 317–329.
23. Wei, H.; Zhao, Z.; Luo, R. Machine-Learned Molecular Surface and Its Application to Implicit Solvent Simulations. J. Chem. Theory Comput. 2021, 17, 6214–6224.
24. Sehnal, D.; Bittrich, S.; Deshpande, M.; Svobodová, R.; Berka, K.; Bazgier, V.; Velankar, S.; Burley, S.K.; Koča, J.; Rose, A.S. Mol* Viewer: Modern web app for 3D visualization and analysis of large biomolecular structures. Nucleic Acids Res. 2021, 49, W431–W437.
25. Goodsell, D.S.; Autin, L.; Olson, A.J. Illustrate: Software for biomolecular illustration. Structure 2019, 27, 1716–1720.
26. Porter, T.K. The shaded surface display of large molecules. In Proceedings of the the 6th Annual Conference on Computer Graphics and Interactive Techniques, Chicago, IL, USA, 8–10 August 1979; pp. 234–236.
27. Moll, A.; Hildebrandt, A.; Lenhof, H.P.; Kohlbacher, O. BALLView: A tool for research and education in molecular modeling. Bioinformatics 2006, 22, 365–366.
28. Stone, J.E. Interactive ray tracing techniques for high-fidelity scientific visualization. In Ray Tracing Gems: High-Quality and Real-Time Rendering with DXR and Other APIs; Apress:

Berkeley, CA, USA, 2019; pp. 493–515.

29. Phong, B.T. Illumination for computer generated pictures. Commun. ACM 1998, 18, 311–317.
30. Blinn, J.F. Models of light reflection for computer synthesized pictures. In Proceedings of the 4th Annual Conference on Computer Graphics and Interactive Techniques, San Jose, CA, USA, 20–22 July 1977; pp. 192–198.
31. Miller, G. Efficient algorithms for local and global accessibility shading. In Proceedings of the the 21st Annual Conference on Computer Graphics and Interactive Techniques, Orlando, FL, USA, 24–29 July 1994; pp. 319–326.
32. Zhukov, S.; Iones, A.; Kronin, G. An ambient light illumination model. In Proceedings of the Rendering Techniques' 98: Proceedings of the Eurographics Workshop, Vienna, Austria, 29 June–1 July 1998; Springer: Berlin/Heidelberg, Germany, 1998; pp. 45–55.
33. Tarini, M.; Cignoni, P.; Montani, C. Ambient occlusion and edge cueing for enhancing real time molecular visualization. IEEE Trans. Vis. Comput. Graph. 2006, 12, 1237–1244.
34. Matthews, N.; Easdon, R.; Kitao, A.; Hayward, S.; Laycock, S. High quality rendering of protein dynamics in space filling mode. J. Mol. Graph. Model. 2017, 78, 158–167.
35. Hermosilla, P.; Vázquez, P.; Vinacua, À.; Ropinski, T. A general illumination model for molecular visualization. Comput. Graph. Forum 2018, 37, 367–378.
36. Zerari, A.E.M.; Babahenini, M.C. Screen space ambient occlusion based multiple importance sampling for real-time rendering. 3D Res. 2017, 9, 1.
37. Lawonn, K.; Viola, I.; Preim, B.; Isenberg, T. A survey of surface-based illustrative rendering for visualization. Comput. Graph. Forum 2018, 37, 205–234.
38. Koch, T.B.; Kouril, D.; Klein, T.; Mindek, P.; Viola, I. Semantic Screen-Space Occlusion for Multiscale Molecular Visualization. In Proceedings of the VCBM@ MICCAI, Granada, Spain, 16–20 September 2018; pp. 197–201.
39. Liang, M.; Fu, Y.; Gao, R.; Wang, Q.; Nie, J. Ellipsoidal abstract and illustrative representations of molecular surfaces. Int. J. Mol. Sci. 2019, 20, 5158.
40. Waldin, N.; Le Muzic, M.; Waldner, M.; Gröller, E.; Goodsell, D.; Ludovic, A.; Viola, I. Chameleon: Dynamic color mapping for multi-scale structural biology models. In Proceedings of the Eurographics Workshop on Visual Computing for Biomedicine, Bergen, Norway, 7–9 September 2016; Volume 2016.
41. Waldin, N.; Waldner, M.; Le Muzic, M.; Gröller, E.; Goodsell, D.S.; Autin, L.; Olson, A.J.; Viola, I. Cuttlefish: Color Mapping for Dynamic Multi-Scale Visualizations. Comput. Graph. Forum 2019, 38, 150–164.

42. Le Muzic, M.; Autin, L.; Parulek, J.; Viola, I. cellVIEW: A tool for illustrative and multi-scale rendering of large biomolecular datasets. In Proceedings of the Eurographics Workshop on Visual Computing for Biomedicine, Chester, UK, 14–15 September 2015; Volume 2015, p. 61.
43. Goodsell, D.S.; Franzen, M.A.; Herman, T. From atoms to cells: Using mesoscale landscapes to construct visual narratives. J. Mol. Biol. 2018, 430, 3954–3968.
44. Garrison, L.; Bruckner, S. Considering best practices in color palettes for molecular visualizations. J. Integr. Bioinform. 2022, 19, 20220016.
45. Guo, D.; Nie, J.; Liang, M.; Wang, Y.; Wang, Y.; Hu, Z. View-dependent level-of-detail abstraction for interactive atomistic visualization of biological structures. Comput. Graph. 2015, 52, 62–71.
46. Miao, H.; Klein, T.; Kouřil, D.; Mindek, P.; Schatz, K.; Gröller, M.E.; Kozlíková, B.; Isenberg, T.; Viola, I. Multiscale molecular visualization. J. Mol. Biol. 2019, 431, 1049–1070.
47. Müller, C.; Braun, M.; Ertl, T. Optimised molecular graphics on the hololens. In Proceedings of the 2019 IEEE Conference on Virtual Reality and 3D User Interfaces (VR), Osaka, Japan, 23–27 March 2019; pp. 97–102.
48. Goddard, T.D.; Brilliant, A.A.; Skillman, T.L.; Vergenz, S.; Tyrwhitt-Drake, J.; Meng, E.C.; Ferrin, T.E. Molecular visualization on the holodeck. J. Mol. Biol. 2018, 430, 3982–3996.
49. Koradi, R.; Billeter, M.; Wüthrich, K. MOLMOL: A program for display and analysis of macromolecular structures. J. Mol. Graph. 1996, 14, 51–55.
50. DeLano, W.L. Pymol: An open-source molecular graphics tool. CCP4 Newsl. Protein Crystallogr. 2002, 40, 82–92.
51. Sterzik, A.; Lichtenberg, N.; Krone, M.; Cunningham, D.W.; Lawonn, K. Perceptual Evaluation of Common Line Variables for Displaying Uncertainty on Molecular Surfaces. In Proceedings of the Eurographics Workshop on Visual Computing for Biology and Medicine, Vienna, Austria, 22–23 September 2022; The Eurographics Association: Eindhoven, The Netherlands, 2022.
52. Sterzik, A.; Lichtenberg, N.; Krone, M.; Baum, D.; Cunningham, D.W.; Lawonn, K. Enhancing molecular visualization: Perceptual evaluation of line variables with application to uncertainty visualization. Comput. Graph. 2023, 114, 401–413.
53. Schulz, C.; Schatz, K.; Krone, M.; Braun, M.; Ertl, T.; Weiskopf, D. Uncertainty visualization for secondary structures of proteins. In Proceedings of the 2018 IEEE Pacific Visualization Symposium (PacificVis), Kobe, Japan, 10–13 April 2018; pp. 96–105.
54. Rheingans, P.; Joshi, S. Visualization of molecules with positional uncertainty. In Proceedings of the Data Visualization’99: Proceedings of the Joint EUROGRAPHICS and IEEE TCVG Symposium on Visualization, Vienna, Austria, 26–28 May 1999; Springer: Berlin/Heidelberg, Germany, 1999; pp. 299–306.

55. Maack, R.G.; Raymer, M.L.; Wischgoll, T.; Hagen, H.; Gillmann, C. A framework for uncertainty-aware visual analytics of proteins. Comput. Graph. 2021, 98, 293–305.
56. Kut'ák, D.; Vázquez, P.P.; Isenberg, T.; Krone, M.; Baaden, M.; Byška, J.; Kozlíková, B.; Miao, H. State of the art of molecular visualization in immersive virtual environments. Comput. Graph. Forum 2023, 42, e14738.
57. Norrby, M.; Grebner, C.; Eriksson, J.; Bostrom, J. Molecular rift: Virtual reality for drug designers. J. Chem. Inf. Model. 2015, 55, 2475–2484.
58. Gebhardt, P.; Yu, X.; Köhn, A.; Sedlmair, M. Molecusense: Using force-feedback gloves for creating and interacting with ball-and-stick molecules in vr. In Proceedings of the 15th International Symposium on Visual Information Communication and Interaction, Chur, Switzerland, 16–18 August 2022; pp. 1–5.
59. KL, N.S.; Chavan, P.S.; Murthy, S. StereoChem: Augmented reality 3D molecular model visualization app for teaching and learning stereochemistry. In Proceedings of the 2018 IEEE 18th International Conference on Advanced Learning Technologies (ICALT), Mumbai, India, 9–13 July 2018; pp. 252–256.
60. Hoog, T.G.; Aufdembrink, L.M.; Gaut, N.J.; Sung, R.J.; Adamala, K.P.; Engelhart, A.E. Rapid deployment of smartphone-based augmented reality tools for field and online education in structural biology. Biochem. Mol. Biol. Educ. 2020, 48, 448–451.
61. Dos Santos Baglie, L.S.; Neto, M.P.; de Paiva Guimarães, M.; Brega, J.R.F. Distributed, immersive and multi-platform molecular visualization for chemistry learning. In Proceedings of the Computational Science and Its Applications–ICCSA 2017: 17th International Conference, Trieste, Italy, 3–6 July 2017; Part I. Springer: Berlin/Heidelberg, Germany, 2017; pp. 569–584.
62. Todd, H.; Emsley, P. Development and assessment of CootVR, a virtual reality computer program for model building. Acta Crystallogr. Sect. D Struct. Biol. 2021, 77, 19–27.

Retrieved from https://encyclopedia.pub/entry/history/show/123940