Dynamic Molecular Principles for Science Animators

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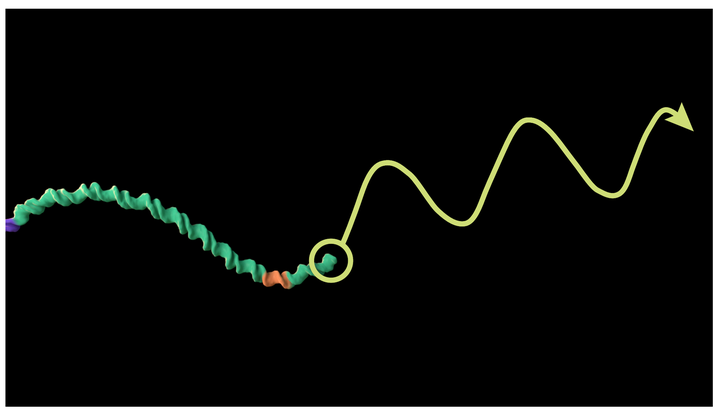
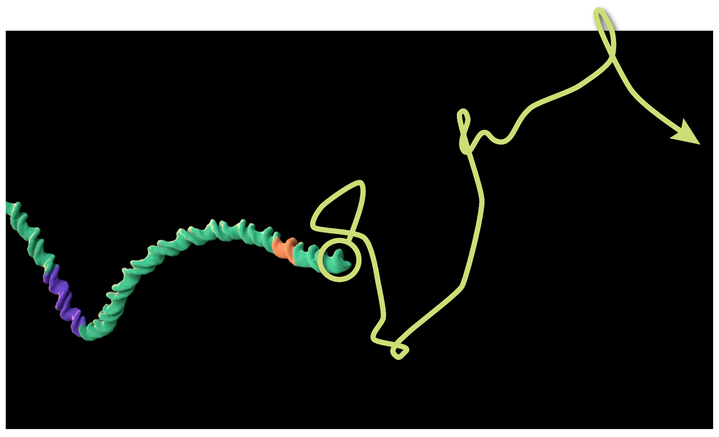
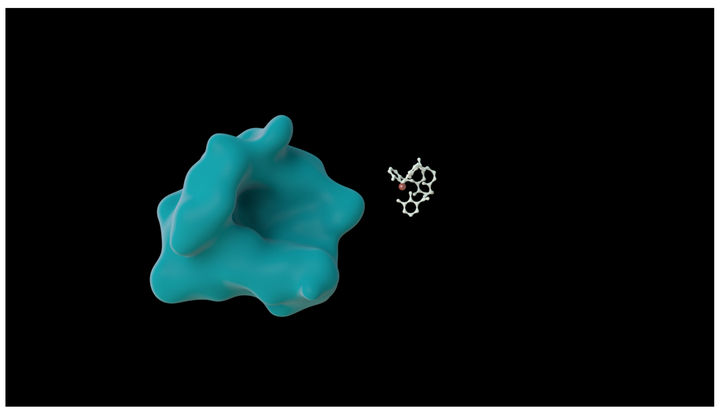


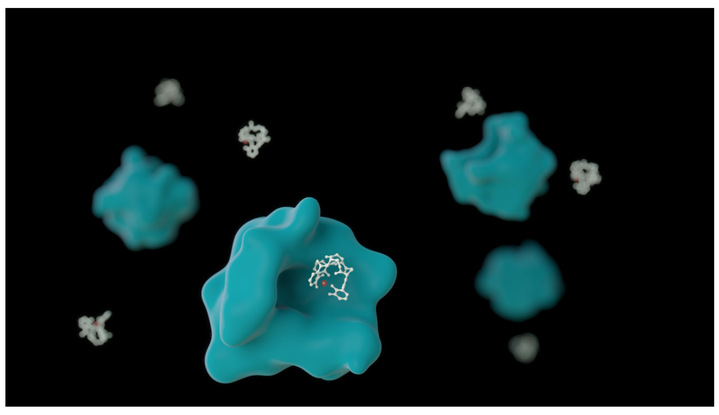
Principle 2: Avoid "snake" motion
Treatment A: Trajectory shows sinusoidal motion



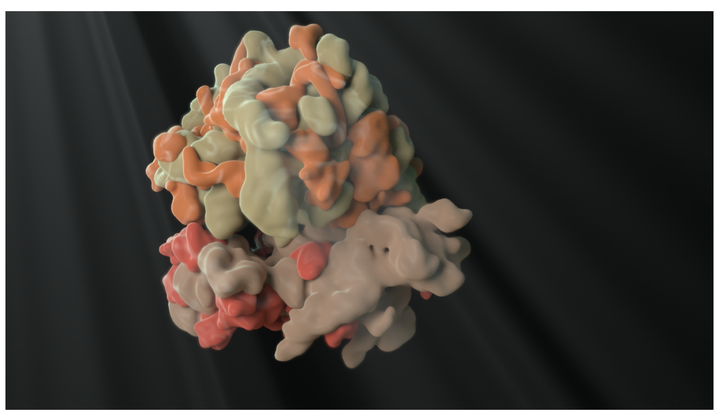
Principle 2: Avoid "snake" motion
Treatment B: Trajectory shows random motion



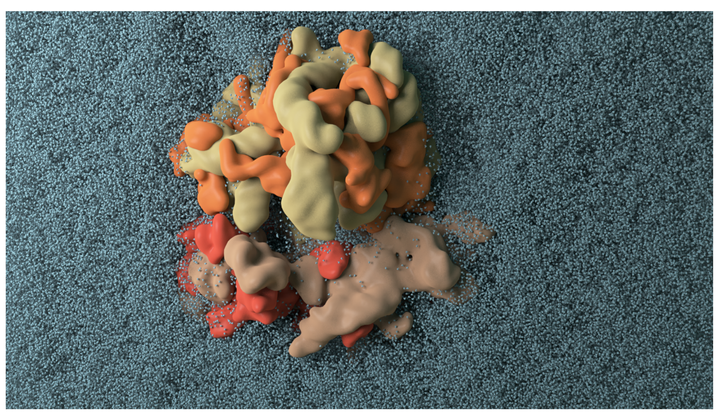
Principle 6: Show multiple copies
Treatment A: A single enterobactin molecule binds to a single siderocalin molecule



Principle 6: Show multiple copies
Treatment B: Several enterobactin molecules bind to several siderocalin molecules



Principle 8: Avoid underwater effects
Treatment A: Ribosome with caustics, ripple distortion, and crepuscular rays



Principle 8: Avoid underwater effects
Treatment B: Ribosome partially surrounded with water molecules at accurate density

Background & Objective

Through our research into how biology students learn from animation, it appears there is often a disconnect between **molecular processes** (e.g. a cell signal cascade) and **behaviours** (e.g. Brownian motion)[1]. Visualizations may help **bridge this gap**[2]. However, because of technical limitations, design constraints, or a lack of awareness of some fundamental concepts, 3D animations can show macromolecules with **biophysically inaccurate properties**.

Science animators must ask themselves, "**How shall I depict molecular motion?**", "**How will these molecules interact?**", and "**How shall I populate the environment?**" We have identified **twelve principles** that serve as reminders of concepts and behaviours. We hope they will encourage designers to consider how to depict molecular phenomena **accurately** while **conveying information clearly**.

Visualization Design

Each principle is presented as a pair of short animations where **Treatment A does not** adhere to the principle and **Treatment B does**. For the sake of **clarity**, each pair depicts a simplified biological example and each principle is presented in isolation from other principles. The rendering style is clean and simple, yet uses plausible molecular representations.

The "Principles"

Note: Order is not of importance. Light gray principles are in production.

1) Use random walks
   Molecules move around through collisions and random Brownian motion.

2) Avoid "snake" motion
   The same forces are present along the length of a long molecule. Putting a head to a molecule invokes agency.

3) Avoid spontaneous starts and stops
   Molecules respect Newton's first law and are in constant motion.

4) Avoid the "vacuum" effect
   There are no long range attractions between interacting molecules; this invokes agency.

5) Add non-binding collisions
   Not every encounter between complementary molecules results in binding.

6) Show multiple copies
   There are typically many instances of molecules and events present in an environment.

7) Leave some behind
   Not every molecule is used in a process or changes its state.

8) Avoid underwater effects
   Light does not behave with macroscopic phenomena at molecular scales. Water is composed of molecules.

9) Avoid sparse/empty environments
   Molecular environments are busy and crowded.

10) Avoid molecules passing through each other
    Molecules are physical entities that experience steric effects.

11) Show protein flexibility
    Proteins have internal freedom of motion that allows for adaptable functionality.

12) Show reversible states and demonstrate equilibrium
    Molecules do not bind permanently and many reactions are reversible at the level of individual molecules.

References & Funding

1. Jenkinson, J., Jantzen, S.G., Gauthier, A., and McGill, G. Examining Students' Understanding of Molecular Interactions Using An Adaptive Assessment Tree. Poster presented at Gordon Research Conference on Visualization in Science & Education. Bates College, Lewiston, ME, USA. August 2–7, 2015.

2. Tasker, R., and Dalton, R. (2008). Visualizing the Molecular World – Design, Evaluation, and Use of Animations. In J. K. Gilbert, M. Reiner, & M. Nakhleh (Eds.), Visualization: Theory and Practice in Science Education (pp. 103–131). Dordrecht, Netherlands: Springer.

All animations can be viewed at our lab website **www.sciencevis.ca**. This research is supported in part by grants NSF #DUE1220512 from the National Science Foundation (USA) and SSHRC #SIG-13/14 from the Social Sciences and Humanities Research Council (CAN).

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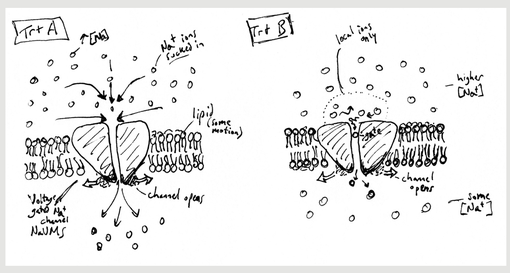
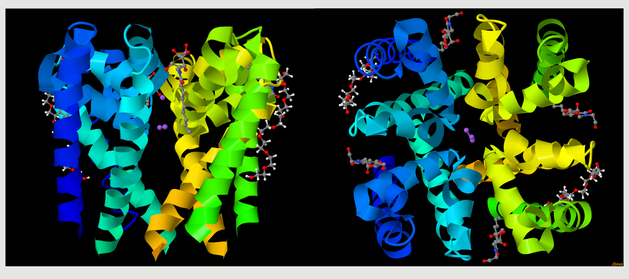
Process

1) Concept development



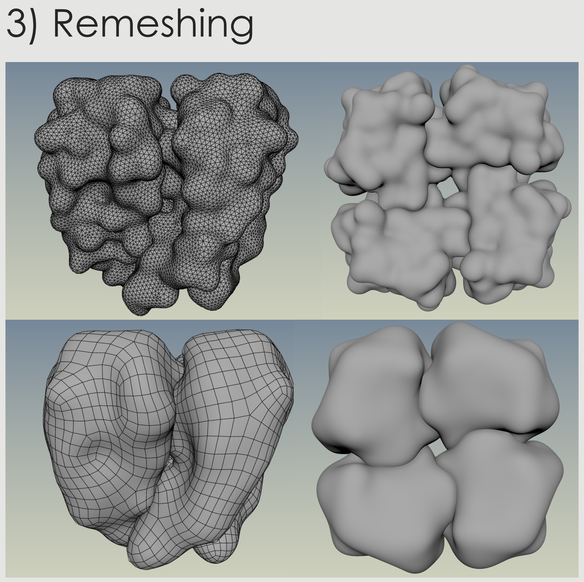
A biological example is chosen for the principle and the plan for presenting both treatments is sketched out.

2) Structural Data



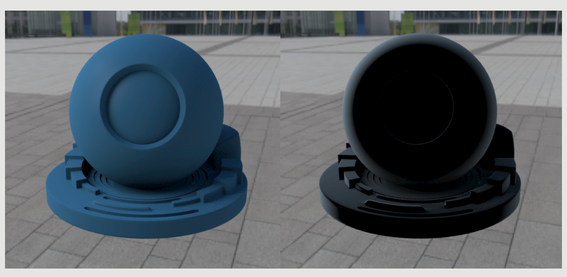
Structural data is taken from the Protein Data Bank, in this case, for NavMs (PDB: 3ZJZ).

3) Remeshing



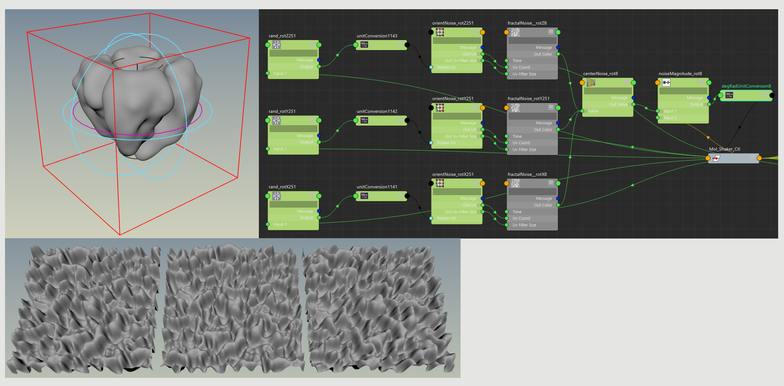
The molecule is meshed and retopologized for a smoother, simpler representation.

4) Light & Shading



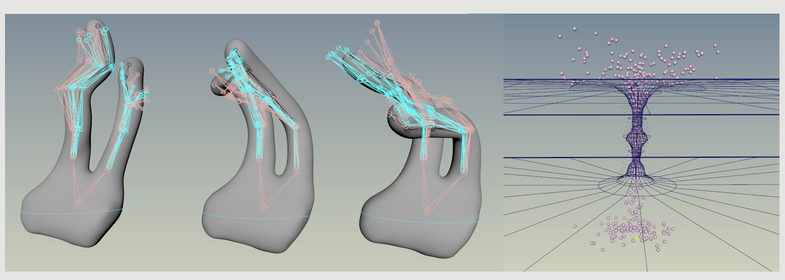
Shaders are designed to be simple, clear, and elegant. A diffuse colored surface combined with a subtle lighter sheen work well for this presentation. Scenes are lit with a large area light and environment sphere.

5) Motion rig



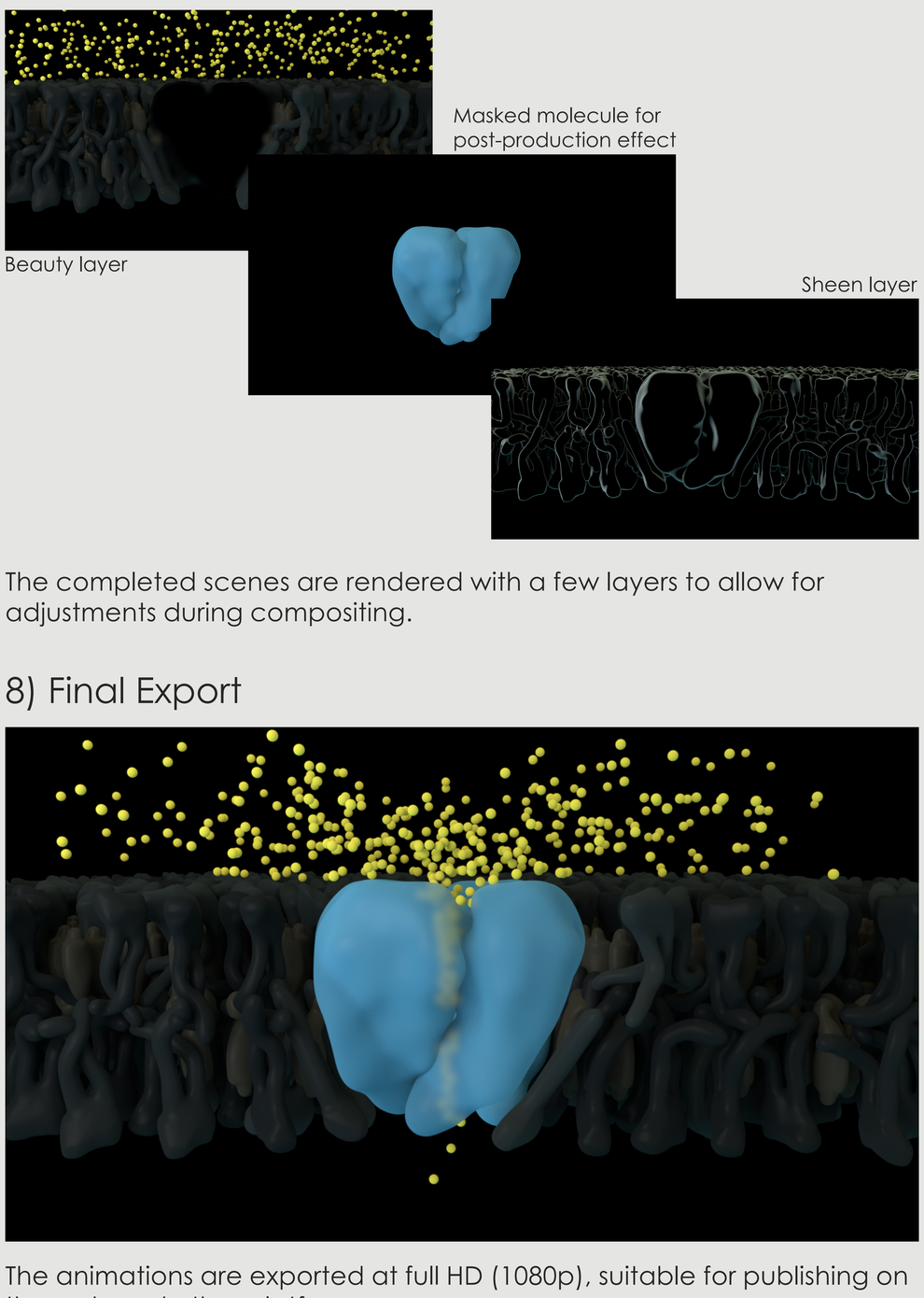
Molecules are rigged for procedural animation using noise textures to drive translation and rotation. Other controls are set up, e.g. for opening the channel.

6) Animation & Simulation



Molecules are animated combining procedural and key-frame animation. Dynamic simulations are run with forces and colliders to control the speed and range of motion.

7) Rendering & Compositing



The completed scenes are rendered with a few layers to allow for adjustments during compositing.

8) Final Export

The animations are exported at full HD (1080p), suitable for publishing on the web and other platforms.