Primer for Visualisation

Primer: A step-by-step guide for visualisation.

The following is a quick start guide using the CrystalGrower visualiser. For more information, please watch the playlist on our YouTube channel.

General Use

1. Load your data (.vis) file (File > Load Data File / CTRL + O).
2. Load your coordinates (.XYZ) file (File > Load Coordinates File / CTRL + SHIFT + O).
3. Manipulate your displayed structure using the mouse and keyboard controls. (WASD, Z and X, left, right and middle mouse buttons).
    a. If the operations are slow, try switching to points mode, manipulate your structure, then switch back. (CTRL + SHIFT + P or Drawing > Structure Type > Points).
4. Try changing drawing modes e.g. layers spheres, tiles etc (Drawing menu)
5. Try resizing spheres or changing custom colours by selecting species. (Spacebar and Colouring menu, CTRL + PLUS and CTRL + MINUS to resize spheres).
6. Save a custom state (.stat) to retain all your changes when reloading the simulation later. (File > Save Current State)
7. Try changing the lighting options. (Lighting menu).
8. If using spheres, increase the resolution of spheres before taking an image. (Drawing > Change Sphere Resolution) then use CTRL + PLUS and CTRL + MINUS to change sphere resolution.
9. Make sure the overlay / axes are either off or display the information you want. (View > Overlay Options and Axes Options)
10. Try moving the depth buffers to look inside the crystal, if internal defects are present. (CTRL + SHIFT, J and K or N and M)
11. Take an image with CTRL + S or using the menu option.

12. If you’re stuck – try the Reset menu options. (CTRL + SHIFT + R will reset to the starting viewpoint).

Making Movies

1. Load your data (.vis) file.
2. Load a multi-frame (or single frame for rotation / flight path movies). This will take a long time for larger simulation files.
3. Use the left, right, up and down arrows to scroll through simulation frames.
4. Use the save all frames menu option to save all simulation frames from your current viewpoint with your custom size, colour and drawing modes loaded. This will create a series of images that can be scrolled through to show the crystal growing over time.
5. For pre-programmed rotations, simply click render movies and select any option from clockwise or anticlockwise.
6. For flight path movies, define a starting and ending viewpoint.
7. Select an option from render movies > flight path.
    a. Enable or disable the direct path calculation, depending on the type of flight you require.
8. Stitch your frames together in editing software (e.g. Windows video editor (free, bundled with Windows 10), Windows Movie Maker (deprecated), Camtasia (paid software), Shotcut (free)).
9. Export your completed movie with your desired quality settings.

High-throughput

1. Prepare your folder with .XYZ files of the same structure (ideally with the same layers / tiles information – although not essential, drawing in layers mode will skip taking images for files that have no layers information). Ensure you perform this on a device with enough storage space.
2. Load your data (.vis) file.
3. Load a coordinates file and set your view position and custom colours etc. Ensure that the view distance is far enough to account for crystals with different morphologies in your folder (especially if your simulation series is over a large range of free energies of crystallisation).
4. Invoke one of the high-throughput commands from the File menu.
5. Wait for the files to finish processing.