

## Multi-Frame Processing and Movies

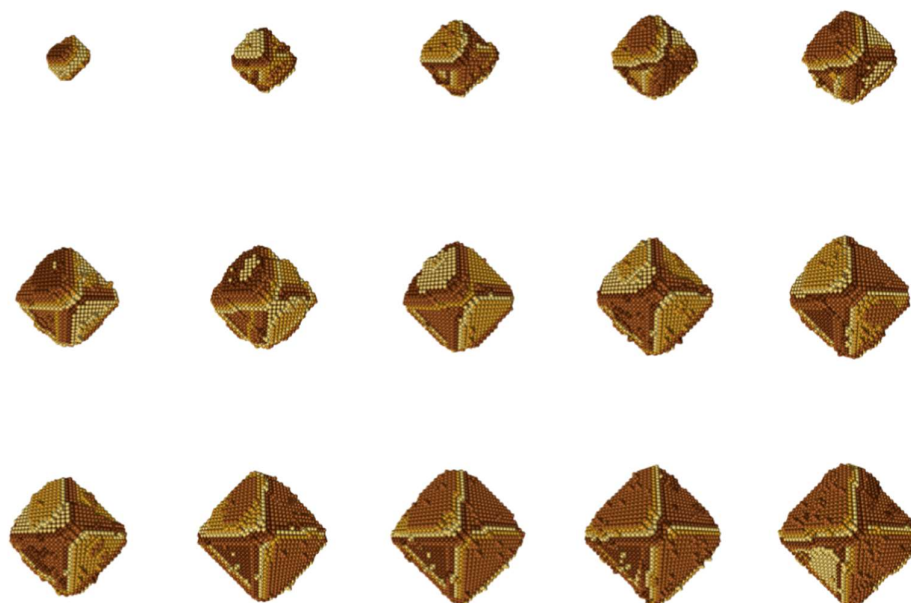
**Movie control:** Multi-frame simulations have extended functionality in the visualiser, allowing users to switch between frames and record sequences of frames as images to show crystal growth or dissolution. Movies can also be generated of single and multi-frame simulations moving in space by rotation or translation to show the crystal habit from multiple angles.

The ability to study simulations of multiple frames was one of the crucial features the visualiser was designed to include from the outset. Currently, the maximum number of frames that can be read into the visualiser is defined by a PC's available memory to store the large numbers of XYZ coordinates contained in these files (this limit is greater in the 64 bit version of the visualiser than the 32 bit version). It is important to note that simulations of multiple frames can rapidly increase the file size of the ".XYZ" coordinate files, which will increase the read in time for the visualiser. Once the read in phase is completed, the speed of manipulation of the simulations results (e.g. rotation and translation) is only dependent on the number of species currently displayed on the screen.

Users are able to view one frame at a time in the visualiser but can switch between individual frames using the LEFT or RIGHT arrow keys. For larger simulations with a high number of frames, users can skip forward or backwards 10 frames at a time with the UP and DOWN arrow keys, respectively. Pressing the "1" or "0" keys skips to either the first or final frame of the simulation, respectively. Simulations of multiple frames are loaded in the same fashion as single frame simulations and have access to all of the aforementioned options. Stills of the simulated growth of a faujasite (FAU) crystal are shown in Figure 14.

Currently, the visualiser is only capable of outputting images as bitmaps. By selecting "File > Save Image" or CTRL + S users are encountered with a file explorer screen allowing them to save an image and assign it a file name. The visualiser saves images by taking a capture of whatever the visualiser window is currently displaying, this leads to file size being dependent on the size (or resolution) of the window. Users can also select the "Save All Frames" option, which will save an image for each simulation frame with the current camera position and colouring / drawing mode. Stitching these images together in video editing software (e.g. Windows Movie Maker (now deprecated), Windows Video Editor (bundled with Windows 10), Camtasia or Shotcut) gives the appearance of movie of how a crystal changes (e.g. growth or dissolution) with simulation time (Figure 14).

In addition to the option of recording movies of growth and dissolution, the visualiser is also capable of creating movies of crystals translating, rotating or a combination of the two, referred to as a “flight path” movie. By selecting the “View” drop-down menu, users can set a beginning and ending point for their movie with “Set Starting Viewpoint” and “Set Ending Viewpoint”, respectively. Movies are generated by subtracting the rotation and translation values for the ending viewpoint from the starting viewpoint and dividing the resulting values by how the number of frames the user wishes to generate. Selecting the “Render Movies” drop-down menu from the visualiser toolbar and highlighting the “Flight Path” option will allow the user access to three movie types. These movie types differ by the order they conduct the translation or rotation steps or conduct both transitions at the same time. Selecting “Rotation, Translation” will conduct the rotational transition in the first half of the generated movie, followed by translation in the second half, whereas this order is reversed for the “Translation, Rotation” option. “Rotation + Translation” differs to these options as the translational and rotational transitions both occur at the same time. Consequently, “Rotation + Translation” movies are generally shorter and are strictly speaking the only true example of a “flight path” within the visualiser. The “Take Most Direct Path” option will allow the visualiser to calculate the most efficient path between two points (e.g. a rotation 315 degrees about Y is far longer than a -45 degree rotation about Y). If users would prefer taking the longer path between points, then this option can be disabled.



**Figure 14:** Still images taken from a multi-frame simulation of the crystal growth of a FAU crystal in layers mode. Starting from the top left and progressing to the bottom right corner, each frame is taken at a different simulation time.

Highlighting either movie type leads to another drop-down menu where the user can specify how many frames (images) they would like their movie to be composed of. The larger the number of frames specified, the smoother transitions will appear when stitching the resulting images together. However, a larger amount of file space will be used to save the increased number of images. As well as the flight path options, users can also select from a set of pre-prepared rotation operations in both the clockwise and anticlockwise directions. These can be produced by selecting the “Rotate Clockwise” and “Rotate Anticlockwise” options under the “Render Movies” drop-down menu, followed by specifying which axis to rotate around from a list of options. Each of these pre-generated rotations records an image every ten degrees of rotation until returning to the point at which the option was selected, giving a total of 37 images. The variety of movie types that can be produced in the visualiser allows users to plot out longer movies combining each of the types together as they desire. Several movies have been produced by combining a number of smaller movies e.g. a flight path to zoom out from a crystal, a movie of the crystal growing followed by another flight path to zoom in on terraces – which can be seen on our website: <https://crystalgrower.org/>.