<u>Memory</u>

Do you want to calculate memory for the simulation?: With "yes" checked *CrystalGrower* will first grow a small crystal and then try to determine how much memory is required to complete the entire simulation. It is not absolutely foolproof but works for most situations and optimises memory allocation. With "no" checked the user will be asked to allocate memory (see next section).

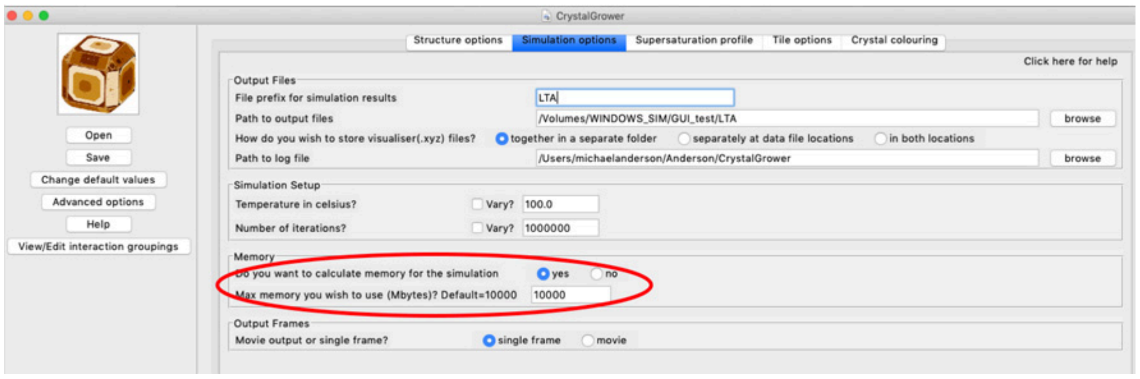
Max memory you wish to use (MBytes)? Default=10000: this option will only appear if users request for memory to be calculated automatically and prevents too much memory being allocated by the automatic memory function should users request a simulation of a very large crystal.

Size of simulation in the x/y/z direction (Must be odd): Only asked if users request for memory to not be automatically calculated. This is the number of unit cells to be assigned to memory in the a, b and c directions of the primitive cell. If this is too small then the simulation will terminate early and save the grown crystal at that point. If a checkpointed file is read in then the size of the simulation will need to be entered.

These three questions define the memory allocated in which to grow the crystal. A 3-dimensional memory box is created that contains x unit cells in the a-direction, y unit cells in the b-direction and z unit cells in the c-direction. It is important, however, to understand that this memory allocation is based upon the primitive unit cell in which the calculation is done. The structure file will indicate the primitive unit cell being used. This memory allocation can be done automatically or manually.

Automatic memory allocation is achieved by answering “yes” to the first question as shown below. Then the answer to the second question is the maximum memory allocation that you wish to allow to be allocated. The default value of 10,000 Mbytes is usually sufficient. If the automatic memory allocation exceeds this maximum memory permitted the simulation will not run.

The automatic memory is determined by running 100,000 iterations at a high supersaturation and then determining how large the memory required is likely to be for the full simulation. This is an estimate,



Output Files
File prefix for simulation results: LTA
Path to output files: /Volumes/WINDOWS_SIM/GUI_test/LTA
How do you wish to store visualiser(.xyz) files? [✓ together in a separate folder] separately at data file locations in both locations
Path to log file: /Users/michaelanderson/Anderson/CrystalGrower

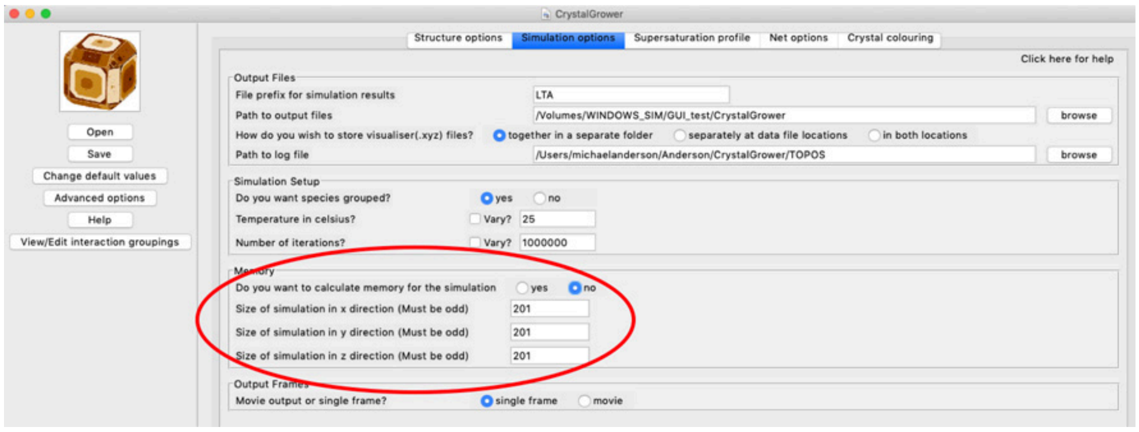
Simulation Setup
Temperature in celsius? Vary? 100.0
Number of iterations? Vary? 1000000

Memory
Do you want to calculate memory for the simulation [✓ yes] no
Max memory you wish to use (Mbytes)? Default=10000: 10000

Output Frames
Movie output or single frame? [✓ single frame] movie

erring on the generous side for the memory allocation. It works for most simulations but is not full-proof. If you have conditions that change dramatically during the simulation it is possible that the simulation will run to the edge of the allocated memory box. In this case the simulation will terminate and the progress output at that point. If the automatic memory allocation does not work for some reason then the first question should be answered "no" and memory allocated manually (see below).

In order to enter the memory allocation manually answer the first question "no" followed by the size of the memory box required. The example below shows an allocation of 201 unit cells in the a, b and c-directions (it does not have to be equal in each direction but the numbers should be odd). If you are loading a checkpointed file then you will have to enter the memory manually. In that case you will be informed of the memory required for the checkpointed file and you can then increase the memory accordingly depending on how many more iterations you conduct.



Output Files

File prefix for simulation results: LTA

Path to output files: /Volumes/WINDOWS_SIM/GUI_test/CrystalGrower

How do you wish to store visualiser(.xyz) files? [✓ together in a separate folder] separately at data file locations in both locations

Path to log file: /Users/michaelanderson/Anderson/CrystalGrower/TOPOS

Simulation Setup

Do you want species grouped? [✓ yes] no

Temperature in celsius? Vary? 25

Number of iterations? Vary? 1000000

Memory

Do you want to calculate memory for the simulation yes [✓ no]

Size of simulation in x direction (Must be odd) 201

Size of simulation in y direction (Must be odd) 201

Size of simulation in z direction (Must be odd) 201

Output Frames

Movie output or single frame? [✓ single frame] movie