Iterations

Number of iterations?: how many (growth + dissolution) steps in the simulation.

The number of iterations defines how many growth + dissolution steps are carried out in the simulation. Every iteration there will be either a growth or a dissolution event. Consequently, the elapsed time between iterations is not constant but can be determined and is reported in the output files "delmu" and "growth". The ultimate size of the crystal will depend on the relative number of growth versus dissolution events. If colouring is turned on then the final size of the crystal is reported in the "simulation_parameters file. Typical values for iterations are: 1,000,000 for a small simulation; 10,000,000 for a medium simulation; 100,000,000 for a large simulation. There is no restriction on this value. However, if you have the automatic memory set in the following question in the GUI then, if the number of iterations is very high, the memory requirement may exceed that available. The memory requirement is evaluated assuming a high supersaturation and therefore only growth with little dissolution. So, the evaluation is erring on the cautious side and, hence, if you set a very high number of iterations but you don't think the crystal will be growing too large, because you expect a lot of dissolution events, it would be better to set the memory size manually.