Saving a Checkpoint File

Do you want to save a checkpoint file?: If you check "yes" then a checkpoint file, which is a record of the simulation, will be saved. This file allows a subsequent simulation to be started from the end of this simulation.

Checkpoint files will be saved with the data files output from a completed simulation (suffix = Simulation_Name_Checkpoint.txt). The write out stage may be slightly slower when producing checkpoint files. Crystals with a large number of internal defects tend to have larger checkpoint files. Once saved, checkpoint files can be loaded as starting points for simulations, provided the crystal structures are both the same and have the same number of site types (i.e. the same grouping answer, and the same answer for multipliers and weighting for multiple bonds).

Please consult the guide on checkpointing to learn how to use checkpoints effectively on our YouTube channel: https://www.youtube.com/channel/UCnftdepWN2iAt_hz8s2WhQg