Checkpoint File

name_checkpoint.txt: this contains information required to restart a *CrystalGrower* simulation from a previous simulation if a checkpoint file save is requested. The file is saved as efficiently as possible but will necessarily contain a substantial amount of information, especially for a large simulation. The checkpoint file can then be read to continue the simulation.

This file can be used to read in a previous file as a seed crystal to begin another simulation. This file repopulates the main grid array (where the crystal is grown) and the sites array (where populations of site types is stored) along with counters to allow the simulation to continue.
Some features are fixed between checkpoints (i.e. anything that affects the number of site types in the program such as weighting and grouping). Poisoning is available across checkpoints but currently, poisons attached to the crystal at the end of the simulation will be lost when starting a new simulation with a checkpoint (although new poisons can then attach).
The file format differs slightly between natural tile and molecular crystals:

Checkpoint – Natural Tile Crystals

No grouping questions or bond weighting questions mean the header lines for a crystal constructed from natural tiles is slightly shorter. The only things that must be fixed are the multiplication method for determining the number of site types in the system and whether the crystal is treated as molecular or natural tiles.

Example

```
Multiplication method from previous simulation:
1
Molecular yes/no answer from previous simulation
no
Grid dimensions:
169 173 173
Previous iterations:
1000000
Number of filled data strips:
2874
Number of growth events:
597896
Previous global time:
 0.11667E+01
Site type populations:
0
2
27
141135

Strip Data:
52 123
1
131
131
```

0
14
0
0

General Example

Multiplication method from previous simulation:
Multiplication method used in the previous simulation for site types
Molecular yes/no answer from previous simulation
Answer to whether the crystal was treated as a molecular crystal in the previous simulation
Grid dimensions:
X Y Z grid dimensions used in the previous simulation to grow the crystal. Automatic memory allocation is disabled after checkpoint loading.
Previous iterations:
Number of iterations at the end of the previous simulation.
Number of filled data strips:
Number of lines across the grid / box where the crystal was grown that contain any grown crystal units.
Number of growth events:
Number of growth events at the end of the previous simulation.
Previous global time:
Time at the end of the previous simulation (1/sum of all probabilities)
Site type populations:
Population of site type
-Repeat for all sites types in the system-

Strip Data:
***Y Z coordinates of data strip (will increment with X)
Number of blocks of data (uninterrupted line of grown crystal unit cells with no bulk unit cells)
** Start of unit cell block in X

```
End of unit cell block in X
* Site type of species in unit cell
                -* Repeat for all species in unit cell-
           -*Repeat for all unit cells in block-
      -**Repeat for all blocks in strip-
-***Repeat for all strips in crystal-
```

Checkpoint – Molecular Crystals

Additional grouping of molecules together by type and bond weighting all affect the number of site types in the simulation and must therefore be fixed between checkpoints, making the start of this checkpoint file slightly longer.

```
Multiplication method from previous simulation:
1
Grouping answer from previous simulation
yes
Molecular yes/no answer from previous simulation
yes
Weighting yes/no answer from previous simulation:
no
Grid dimensions:
169 173 173
Previous iterations:
1000000
Number of filled data strips:
2874
Number of growth events:
597896
Previous global time:
 0.11667E+01
Site type populations:
0
2
27
141135

Strip Data:
52 123
1
```

131
131
0
14
0
0

General Example

Multiplication method from previous simulation:
Multiplication method used in the previous simulation for site types
Molecular yes/no answer from previous simulation
Answer to whether the crystal was treated as a molecular crystal in the previous simulation
Grouping answer from previous simulation
Answer to whether molecules were grouped by type in the previous simulation
Weighting yes/no answer from previous simulation:
Answer to whether additional bond weighting was used in the previous simulation
Grid dimensions:
X Y Z grid dimensions used in the previous simulation to grow the crystal. Automatic memory allocation is disabled after checkpoint loading.
Previous iterations:
Number of iterations at the end of the previous simulation.
Number of filled data strips:
Number of lines across the grid / box where the crystal was grown that contain any grown crystal units.
Number of growth events:
Number of growth events at the end of the previous simulation.
Previous global time:
Time at the end of the previous simulation (1/sum of all probabilities)
Site type populations:

Population of site type
-Repeat for all sites types in the system-

Strip Data:
***Y Z coordinates of data strip (will increment with X)
Number of blocks of data (uninterrupted line of grown crystal unit cells with no bulk unit cells)
** Start of unit cell block in X
End of unit cell block in X
* Site type of species in unit cell
-* Repeat for all species in unit cell-
-*Repeat for all unit cells in block-
-**Repeat for all blocks in strip-
-***Repeat for all strips in crystal-