ColorBARS Help

General settings

- **Parent directory**: Specifies the directory containing all files of interest. The selected folder will be searched for .Dpd_par (DPD input parameter) files and .mtd (DPD output) files.
    - For example, in Figure 1 below, the selected "Documents" folder in the folder selection dialog indicates that the "RI=2-10", "RI=4-8", "RI=6-6", "RI=8-4", and "RI=10-2" folders will all be searched, as well as all subfolders that they contain.
    - If the "RI=2-10" folder were selected instead in the selection dialog, only its subfolders would be searched; the "RI=4-8" folder and all other folders at the same depth as the selected folder would be excluded.

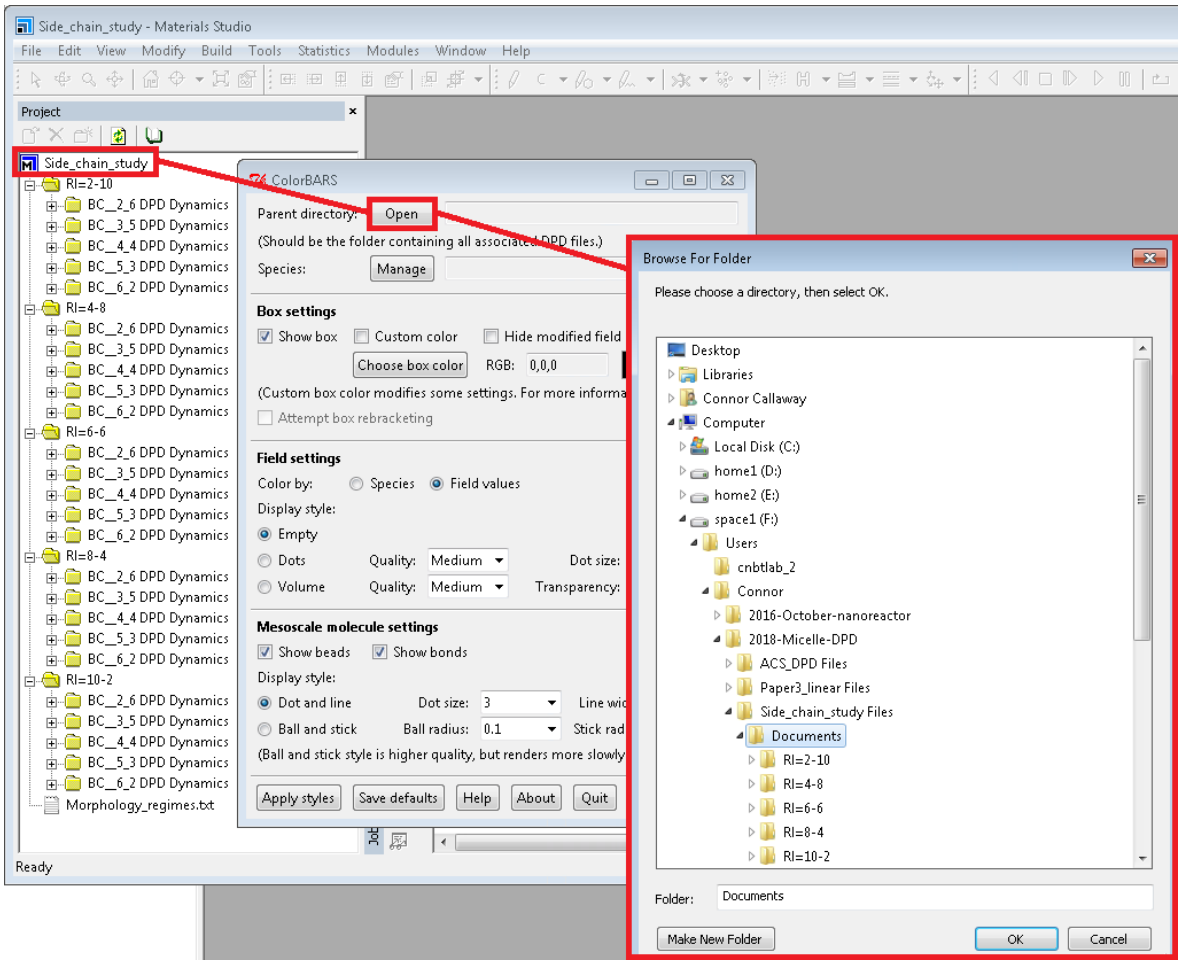

Figure 1. Selecting the “Documents” folder of the Side_chain_study project will search through all subfolders for .Dpd_par and .mtd files.

- As the specified folder and its contents are searched, .Dpd_par files will be read in order to build the species list. If a species is not found in a .Dpd_par file in the specified folder, it will not be available for customization, and ColorBARS will not process it. For this reason, it is not recommended to separate .Dpd_par files from their corresponding .mtd files.
- If no .Dpd_par files are found, the species list will remain empty and no processing will be possible. If no .mtd files are found, attempting to apply the selected styles will have no effect.
- Once the species list has been built, the species manager can be opened by selecting the "Manage" button. A message will appear in the terminal window indicating that file searching is

complete, as shown in Figure 2. From this point on, the specified file path will be designated within ColorBARS as "(…)" for all files.

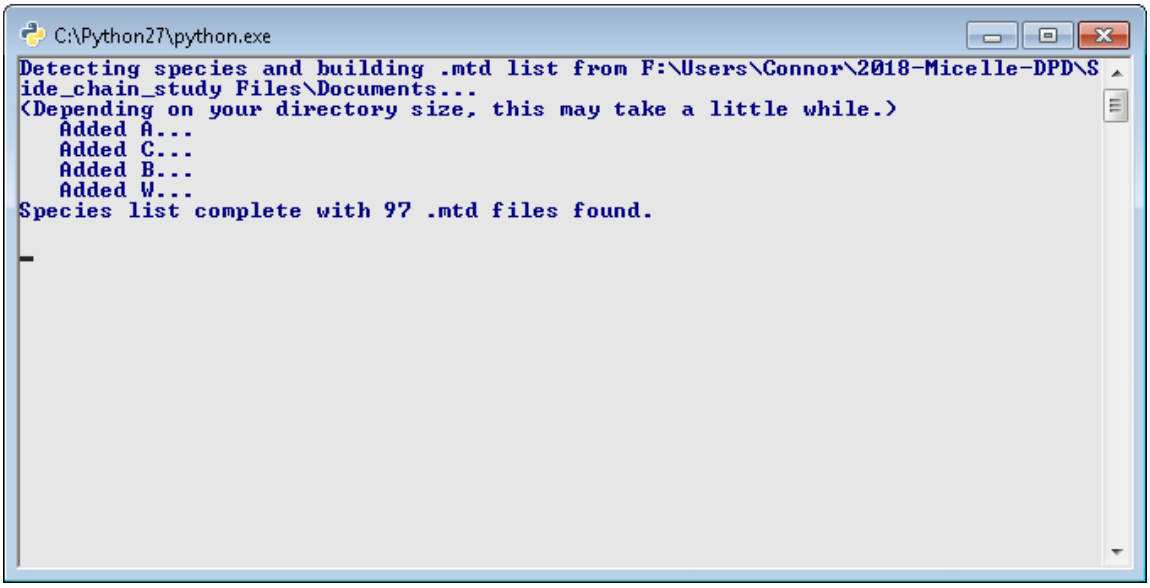

Figure 2. File searching has successfully completed for the specified folder.

- **Manage**: Opens the species manager.
  - A sample species manager for the above system is shown in Figure 3 below.

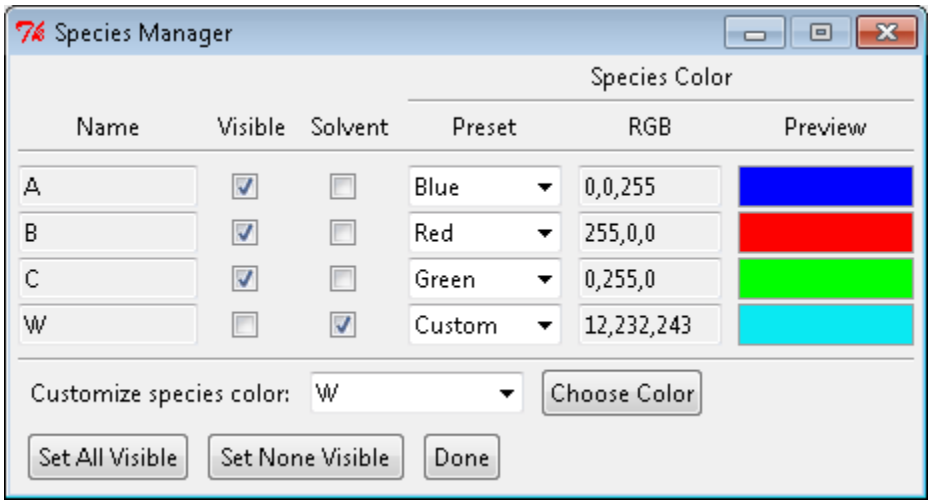

Figure 3. Species manager for a system containing bead names A, B, C, and W. The bead visibility of W is turned off and this bead type is also marked as a solvent species. Preset colors have been selected from the drop-down list for species A, B, and C, while a custom color has been chosen for the W species.

  - The visibility of each species can be independently toggled on or off. If the species visibility is toggled off, that bead type will not be visible in the field display mode or the mesoscale molecule display mode within Materials Studio. The visibility setting of all beads can be toggled on or off via the buttons at the lower left of the species manager.
  - Each species can be marked as a solvent bead type. This affects whether the species will be considered during automatic box rebracketing, discussed later in this guide. At least one solvent species is required to attempt box rebracketing, although if all species are marked as solvents, box rebracketing will be disabled. Further information regarding this method is discussed in that setting's entry in this guide.

- The color of each species can be controlled independently. A selection of preset colors are available, with the corresponding RGB values and a dynamic preview of each color provided as well. If a custom color is desired, select the relevant species from the drop-down list below the species list and select "Choose Color".
- The main ColorBARS window interactivity is disabled while the species manager is open. When satisfied with the species manager settings, close it to restore ColorBARS interactivity.

Box settings

- **Show box**: Toggles the main DPD box visibility on or off.
- **Custom color**: If enabled, allows a custom box color to be specified using the "Choose box color" button below. The RGB value and a dynamic preview of the selected color are also provided below.
- **Hide modified field species**: If enabled, disables the visibility of the last species in the .mtd file. This may not be the same as the last species in the species manager.
  - Materials Studio determines the color of the DPD box via the last species which does not have visibility disabled in the corresponding FloatField block of the .mtd file.
  - As a consequence, customizing the color of the DPD box requires changing the color of the last visible block in the .mtd file. If this option is enabled, ColorBARS will set the field display style of the final species in the .mtd to "Empty" with visibility disabled, so that the color of the box can be customized without forcing the color to be displayed in the system itself.
  - A color can be specified for the affected species in the species manager while still customizing the box color. However, the specified color will be viewable only through the bead view mode, not through the field view mode.
- **Attempt box rebracketing**: If enabled, ColorBARS will attempt to eliminate cutoff bonds at box boundaries for all .mtd files found by re-centering the non-solvent mesomolecular structures in the .mtd file. This option is enabled by default if at least one species is marked as a solvent in the species manager and will likewise be disabled if zero or all species are marked as solvents.
  - If mesomolecules in an .mtd file are found to have mixed solvent and non-solvent beads within their associated topology, these mesomolecules will be excluded during rebracketing and an error message will be displayed in the terminal window.
  - The procedure of box rebracketing relies on the periodic nature of DPD systems. The method will always produce a box of normalized side lengths 1, so a full repeat unit of the system will be maintained. In general, the rebracketing procedure will seek a box boundary position that severs no bonds, effectively shifting atoms to the opposite side of the box if necessary.
  - If an optimal division point is present (i.e., if there exists a box boundary position that severs no bonds), the procedure will nearly always find it. However, some systems may not contain any such division points. In these systems, the rebracketing method will find the division point which severs the fewest number of bonds.
  - Lastly, because the field display mode (see the following section for further information) renders the system using dots representing the relevant field values at various points instead of bonded beads, the box rebracketing procedure will not affect the field display style.

Field settings

The field display mode is one of the two possible display modes for a DPD results file, corresponding to the first tab of the "Display Style" dialog accessible by right-clicking within an open .mtd file. The two display modes are not mutually exclusive, but it is generally more useful to view only one at a time.

- **Color by**: Specifies coloring mode of the field display.
    - **Coloring by species** will use the colors specified within the species manager.
    - **Coloring by field values** will use the settings specified on the "Color Maps" dialog (also accessible via right-click in an open .mtd file).
- **Display style**: Specifies the visual style of the field display. This setting can also be freely changed via the "Display Style" window in Materials Studio.
    - Selecting **Empty** will result in no species being displayed. This is useful if only the mesoscale molecule display mode is desired.
    - Selecting **Dots** will result in the field values being plotted in the .mtd file as a collection of dots. The visual quality and size of these dots may be controlled using the drop-down menus. Figure 4(a) shows a system using the "Dots" display style with quality set to "Medium" and a dot size of 3.
    - Selecting **Volume** will result in the field values being plotted in the .mtd file as continuous regions of color. The visual quality and transparency of these regions may be controlled using the drop-down menus. Figure 4(b) shows a system using the "Volume" display style with quality set to "Low" and transparency set to 75%. The "Volume" display style takes significantly longer to render in most cases.

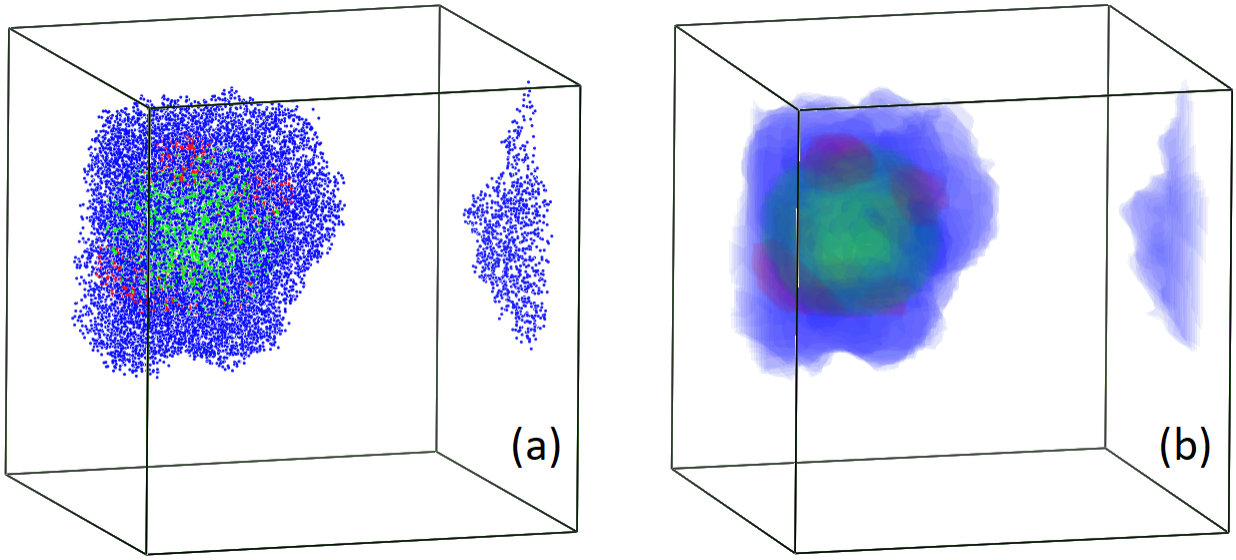

Figure 4. A sample DPD results file using the field display mode (with solvent visibility disabled). (a) The results file is using the "Dots" display style with "Medium" quality and a dot size of 3. (b) The results file is using the "Volume" display style with "Low" quality and transparency of 75%.

- **Note**: <u>The box rebracketing procedure will not affect the field display mode!</u> This can be seen in Figure 4, where both (a) and (b) display a cutoff portion where the mesomolecular structure (in this case, a micelle) crosses the box boundary.

Mesoscale molecule settings

End options

These options refer to the five buttons at the bottom of the ColorBARS interface.

- **Apply styles**: Once all desired settings have been customized, this button apply the settings to all .mtd files found when initially searching the specified file path.

    - A new message in the terminal window will be displayed every time the active .mtd file changes. The common file path (i.e., the path specified as the parent directory at the top of the ColoBARS interface) will be designated as "(…)" for brevity.
    - Additionally, progress updates and estimates of the remaining time until completion will be provided every 10% of the way through the .mtd file list.
- **Save defaults**: Store all currently selected settings into a user-specific configuration file located in the specified BARS Suite GitHub folder.
- **Help**: Opens this document.
- **About**: Provides information about the BARS Suite, the functionality of this entry, and the individuals who contributed to the BARS Suite.
- **Quit**: Close ColorBARS. The window can be closed through other normal means with no risk posed to the program.