Changes to PhreePlot

2015

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31 December 2015 Version 1

- In line with the naming convention for other output files like `*.log`, the `phreeqcall.out` filename has been changed to `<rootfilename>.all` where `<rootfilename>` is the full path to the input file without the extension. The keyword, phreeqcall.out, has also been changed to 'all' although phreeqcall.out remains as an alias. This means that several different `*.all` files can now co-exist in the same directory. It is possible to keep the original `phreeqcall.out` file name by appending this to the 'all' keyword string, e.g. all T `phreeqcall.out`.
- A new keyword, writePlaceholder, was introduced. If TRUE, the default, then a placeholder (the UNDEFINED number, -99999.00) is introduced in the out and trk files when a calculation is skipped or when Phreeqc fails to converge. If FALSE, which can also be useful, no such placeholder is written.
- Revised the indexing of runs so that there is now a master reference number for each run of Phreeqc. This numbering increments by one as each block of Phreeqc code is executed. This includes pre-loop simulations as well as main loop simulations. This makes it easier to uniquely identify a block of code and cross-reference it to that in the *.all file. This reference number is returned by the system tag <nexecute>.
- The keyword, speciationProgramVersion, is now set to blank by default as version information is now obtained directly by querying the Phreeqc library. Any text in speciationProgramVersion is appended to the version string derived from the library.
- The keyword, dateDatabase, is no longer used as this is automatically set to the last date that the database file was modified as read from the database file itself.
- Updated to Phreeqc_3.3.3_svn_10588.

24 August 2015 Version 1

- On some problems with many iterations, the calculations gradually slowed down. This was traced back to a possible compiler error. A workaround has been implemented.

19 August 2015 Version 1

- checkForUpdate was not working properly. Fixed.

18 August 2015 Version 1

- The changes to the clipping made in the previous update introduced a couple of errors detailed below which have been fixed.
- When only a part of the domain of a predominance or contour plot was plotted (e.g.by using pymin, pymax etc), the lines were not clipped at the reduced domain (plot) boundary.
- Also, restoring the Postscript graphic state necessary for turning clipping on/off also restored the previous font size which meant that the text size of a contour legend was not always the correct size.

- Updated the installation instructions to take into account of the new method of producing pdf's introduced in Jan 2014 and in this release, epsi files. The Ghostscript lib and bin directories no longer need to be in the Path.
- A new 'fix anything' example, Al-pH-Ft.ppi, has been put in the '\demo\fix_anything' directory. This draws an Al predominance diagram as a function of total F and pH.
- The Environment variable, PHREEPLOT_PATH, is now set on installation. It points to the directory containing the PhreePlot executable, pp.exe, e.g. C:\Program Files\PhreePlot\. It can be useful in batch files, %PHREEPLOT_PATH%pp xyz.ppi, if the PATH to it has not been set.

28 July 2015 Version 1

- A bug was introduced in the last release affecting the opening of files. The file name printed was sometimes gibberish. Fixed.

21 July 2015 Version 1

- Ghostscript 9.16 (or later) is now the required version of Ghostscript. All previous issues with earlier versions of Ghostscript appear to have been resolved including the new method for creating eps files using the eps2write device rather than the earlier epswrite device. This version of PhreePlot uses this new device and so ideally you will need 9.16 to be installed to create eps files. The original device is still available for GS versions 9.14 and earlier by appending 'old' to the eps line, e.g. 'eps T old' although this is not always reliable at getting the bounding box correct, e.g. when subscripted text is present. If you install Version 9.16, remember to update the pdfMaker setting in pp.set and the /bin and /lib paths in your PATH settings.
- The drawing of lines and symbols using an extraSymbolLines file has been improved (see the Guide). The ends and joins of multiline segments are now rounded (though single line segments are still square butted). It is now also possible to define the line type and dashes per inch for individual line segments as well as turning clipping on and off at will. All line and symbol properties now remain in force until redefined. This may change the behaviour from earlier versions.
- If pageOrientation was set to 1 (landscape), the xoffset on the printed page assumed a page width of 8.5” (i.e. letter size) rather than the specified width. Fixed.
- Recast the demo\AssorptionvspH examples to fix the dissolved P concentration using a generic, 'fix-anything' approach.
- Permissions granted by the installer were extended to the Group 'Everyone' rather than just 'Authenticated Users'. This allows Guest logins to access PhreePlot.
- Updated to Phreeqc_3.2.0_svn_10008.

8 May 2015 Version 1

- Where the input consists of more than one main loop simulation and the *oneSimulationAtATime* option has been selected (e.g. `mainLoop 1 TRUE`), the selected output is now only written to the 'out' file for the last simulation, as originally intended.
- The error reporting has been improved. In the case of a failure of Phreeqc to converge, the Phreeqc output was usually echoed to the screen (except for predominance plots). This now only happens for debug > 0 although the output is still sent to the log file.

- A new system tag, <phreeqc_status_0>, is automatically updated after each run of Phreeqc to indicate the exit status from Phreeqc. 0 is the normal exit; >0 indicates an error with 1 (failure to converge) being the most common.
- A new keyword, stopOnFail, has been added to control what happens when Phreeqc fails: 0 = continue; 1 = stop; 2 = auto (i.e. let PhreePlot decide). The default is 2.
- debug =1 was not stopping predominance calculations immediately after a failure in speciation as indicated in the guide (though debug = 2 was). Reset 1 to stop immediately.
- The sign of the loop increment for the input pre-processor is no longer significant.

28 January 2015 Version 1

- Fixed a regression in which the field boundaries in 'grid' plots were not being drawn properly.
- Updated to Phreeqc_3.1.7_svn_9213.

26 January 2015 Version 1

- The length of the path to the database file was limited to 80 characters not 260. Fixed.
- Updated to Phreeqc 3.1.6 svn 9191.