

Changes to PhreePlot

2013

11 December 2013

Version 1

- A new choice of optimization algorithm has been added for fitting – the Levenberg-Marquadt ('lm') method.
- The track file optionally produced during fitting now contains the elapsed time so that convergence can now be plotted against time.
- fitStepSize is now an alias for fitMaxStepSize and is the preferred form since this more accurately reflects the variable role of this parameter.
- extraSymbolsLines now takes an extra optional parameter – the data separator for the file, e.g “\t” for tabs.
- added a new keyword, useLabelsFile, to prevent edits to the labels file being overwritten and labels repositioned with calculationMethod 1.

6 December 2013

Version 1

- The keyword, checkForUpdate, was added. If true, this checks the PhreePlot website to see if the current version is the most recent (experimental). The default is false.

3 December 2013

Version 1

- A regression crept in on 8 July 2013 that made the TSS, and consequently R2, for fits lower than they should have been (though the RSS, fitted parameter values, standard deviations, plots etc were still correct). Fixed.
- The new unconstrained optimization procedure, 'subplx', a subspace-searching simplex method devised by Tom Rowan, has been added. However, 'nlls' remains the preferred procedure in most cases.
- 'fitMethod' can now take a list of procedures so that different optimization procedures can be tested on the same data set and with the same settings. Also the track (trk) file now records the convergence during fitting (see demo\fit\iso_multifitmethod.ppi).
- Keyword hinting has been introduced for misspelt keywords.

22 November 2013

Version 1

- Was complaining about trailing tabs on 'include' filenames. Fixed.
- Sometimes with multiply-used tags gave an incorrect warning of an undefined tag and failed to set correct tag. Fixed.
- If requested, a plot is now produced during fitting after an interrupt ('Esc') has been issued.

- If the PhreePlot executable (pp.exe) is launched without a command line argument, then besides the normal advisory paragraph, the PhreePlot server is checked to see if there is an update available.

10 November 2013

Version 1

- Fixed an array bounds error that could occur when plotting predominance diagrams.

12 September 2013

- There was sometimes a problem estimating the boundary box for the ps->eps file conversions. This has been fixed.
- The png and jpg keywords now have an optional second parameter that controls the resolution of the image conversion (default = 300 dpi).
- The pts file for the ht1 predominance plot is no longer binary but is formatted (and therefore readable in a text editor).
- Contrary to earlier reports, unrecognised keywords are still treated as fatal errors but this behaviour can be changed with the new unrecognisedKeywordIsFatal keyword.

22 August 2013

- The runtime library, libiomp5md.dll, has been added to the installer.

21 August 2013

Version 1

- PHREEQC has been updated to Version 3.0, a major update.
- Two new keywords, phreeqc.0.out and phreeqc.all.out, have been added to explicitly turn on/off output to the standard PHREEQC output file (phreeqc.0.out) and to the accumulated PHREEQC output file (phreeqc.all.out). Options are 'TRUE', 'FALSE' or 'auto'. If, 'auto', the default, the behaviour is the same as before. Adding these keywords means that the debug keyword no longer has to be used to control these aspects of PHREEQC output.
- Ghostscript 9.07 or later is now the recommended version. The version of Ghostscript used by PhreePlot is determined by the pdfMaker setting in pp.set. It is important that the pdfMaker setting always matches the Path setting for the Ghostscript bin and lib directories - so change them all at the same time. Automatic searching for the Ghostscript executables has been disabled - it was very slow as it searched the whole home drive.
- The PHREEQC module has changed the name of its output files to include the thread number, e.g. phreeqc.0.out, phreeqc.0.err, etc rather than phreeqc.out, phreeqc.err, etc. PhreePlot currently works only on thread 0. PhreePlot file names have been modified to reflect this change.
- Label placement during a 'progress' plot of a predominance plot made with the 'grid' method and using the Eh scale was off target. There were also occasional stray lines in the 'progress' plot - this occurred when the pe was unknown. These

regressions have been fixed.

- Where the same tag had been used and redefined in several places in the PhreePlot section of an input file, the updating sequence was not necessarily in the correct order. Fixed.
- When the summary statistics for the 'carry' variables of a predominance plot were being calculated, the header line was skipped twice resulting in one too few instances. Fixed.
- There was sometimes memory overflow when running a 'custom' calculation in 2D. Fixed.
- There was a fatal error when adding symbols or lines to two or more predominance plots using an extradat file. Fixed.
- A regression meant that ht1s.inc and ht1stability.inc no longer added '(s)' to mineral names as they should have done. Fixed.
- The symbol type was not always read properly from the lineColorDictionary. Fixed.
- The optional -end's have been removed from all supplied BASIC inc files so that it is now possible to add additions and edits to these files in an immediately following inc file (see e.g. ht1s.inc).
- Tags can now be used in the PhreePlot section of an input file (i.e. before CHEMISTRY) as well as in the Chemistry section.
- Plotted lines in custom plots can now have a variety of line styles (dash-dot patterns). These lists are defined by the lineType and dashesPerInch keywords.
- Improvements in the axis tick marks and grid lines. The tickSize keyword (alias tickLength) has been extended to take up to six numbers which define tick lengths for the major and minor x-axis ticks, the major and minor y-axis ticks, and the major and minor 2y-axis ticks. It can also specify whether the ticks are placed inside the axis line or outside it.
- New keywords, gridLines and gridColor now specify whether grid lines are drawn and their colour. gridLineType and gridDashesPerInch define whether the grid line is dashed or not, and the appearance of dashed grid lines.
- A second parameter has been added to the labelEffort keyword which provides an upper limit to the optimization time (in sec) for label placement in custom plots.
- Quite a few enhancements have been made to the contour plot.
- Many of the internal arrays used in preparing a contour plot are now dynamically allocated which means that these plots can deal with more complex figures than before.
- The equally-spaced or 'empirical' method (auto 17 e) for automatically choosing contour values is now the default rather than the 'percentile' option - it is less likely to choose degenerate values.
- A lines-only contour plot which only plots the contour lines, rather than both lines and colour fills, has been introduced. This lines-only plot is easier and quicker to compute since it does not require sorting of line segments or polygon closure, which can sometimes be difficult. It can be selected using a new keyword, contourOptions fill FALSE. The setting contourOptions joinSegments TRUE|FALSE also specifies whether the lines are drawn as a continuous line (with appropriate pretty line joins) or simply as a series of unsorted line segments –

this provides the simplest and most reliable of plots – but not the prettiest.

- There were some problems closing polygons in awkward edge (literally) cases which meant that the colour fill had to be abandoned. This was especially true for low resolution plots. This has been improved and where problems persist, the lines-only option is now available.
- Automatically-generated legends have been added to both line- and fill-type contour plots. Turn off by setting legendTextSize to 0.0.
- There is now an option to smooth the contour z-data before contouring.
- The number of auto-generated fill colours for contour plots has been increased from 18 to 72.
- The labels file is no longer written by a contour plot and the 'f' option for shifting a label using the labels file has been removed. Use one of the other mechanisms provided for moving labels along a contour.
- Added the system tag <systemtime> which records the elapsed time in secs with a granularity of about a microsecond.
- See the demo\contour\contour_timing.ppi for an example demonstrating many of these new features.
- It is now possible to dynamically format numbers in plots written by text strings. The number of significant figures is specified by appending an underscore followed by the number of significant figures wanted, e.g. "1.73946E-3_4" as a text string will plot as 0.001739. This exponent-free notation can be used in any text strings, e.g. in titles, extraText etc and is useful for formatting plotted tag values. Alternatively, if an exponent (E) format is wanted, use \$ instead of _, i.e. "1.73946E-3\$4" will give "1.739E-03". The default (no _ or \$) is 3 significant figures.
- If possible, numeric tag values will be substituted as fixed formal numbers (e.g. 21.13) rather than in an exponent format (e.g. 2.11E01). This enables them to be used in Phreeqc formulae. Exceptions are when the magnitudes are less than 1e-4 or greater than about 1e4. This default behaviour can be overruled with the underscore notation described above.
- 'Include' files are now allowed in the PhreePlot part of an input file, i.e. that part before CHEMISTRY.
- It is now illegal to use one of the 'reserved' system names (x_axis, y-axis, loop etc) as a column heading in the selected output. This avoids inadvertently redefining the tag value associated with these tags.
- Rather than writing reformatted input files to the end of the log file as previously, the input files, including comments, are printed at the beginning of the log file. The keyword, writeAllInputFiles, controls whether just the main input file is printed or all input files including 'include' files. This replaces the rewriteInputFile keyword.
- The keyword, ppa, is no longer used.
- Fitting - it is now possible to produce a contour plot of the (weighted) residual sum of squares as a function of two variables, e.g. two of the model parameters being fitted. This is done by setting calculationType to 'fit' and fitMethod to 'contour', defining the two axis variables with <x_axis> and <y_axis> tags, defining the x- and y-domains with xmin, xmax etc, and defining the contourZvariable as 'rss' or similar. See the example demo\fit\contour_rss.ppi.
- Negative R2 values for a fit no longer signal an error.

- A new keyword, plotOrder, controls the order of plotting lines and points in custom plots.
- A new keyword, legendBox has been added which adds a legend box to custom and contour legends.
- Filenames can now have spaces in them without being quoted.
- A loop file with a single column of character variables will now loop over these variables.
- The PhreePlot guide has been updated.

21 March 2012

Version 1

- Corrected a bug in the contour plotting.

20 March 2012

Version 1

- The number of PHREEQC simulations in an input file is estimated by counting the number of END's. A bug meant that only END's written in all upper case were counted - this has been corrected so that it is now case insensitive as intended.
- A new keyword, omitAccumulate, has been introduced to filter out from execution all PHREEQC lines containing any of one or more specified strings, e.g. 'UNDEFINED'.
- The optional logical switch, oneSimulationAtaTime, associated with the mainLoop keyword was documented but not implemented - it now has been. This switch determines if the mainLoop simulations are run all at once or separately, one at a time.
- The values of 'carry' variables PUNCH'ed while calculating predominance/stability diagrams are now added to the tag dictionary and so can be used in later simulations.
- 'Carry' variables are now added to the tag dictionary even in pre-loop calculations.
- A couple of new ways of drawing mineral stability diagrams are explored in the minstab demos. One is based on not allowing any minerals to precipitate and plotting the field with the highest saturation index (SI) greater than zero. See demo\minstab\minstab2.ppi. The other automatically includes all possible minerals in the EQUILIBRIUM_PHASES data block. See demo\minstab\allminerals.ppi.
- A change to the way that the mainLoop keyword works during fitting has been made. Pre-loop simulations during fitting now only execute once per run, at the beginning (not once per iteration as before). The default setting of mainLoop has also been set to 'auto' rather than 'last'. This 'auto' value is set to 1 for calculationType's 'fit' and 'simulate' and to the 'last' simulation for the other calculation types.
- The occasional unwelcome replacement of a label name by 'NA' during a replot (plotMethod = 3) of a predominance plot has been fixed.
- Improvement in the positioning of multi-line labels.
- Limitations on the length of character strings have been removed from almost everywhere including tag names. This has required adjusting the format of some

of the output files and tables that include labels, tag names and expressions, e.g. the labels and log files. However, all the old format files can still be read. Long names and expressions are sometimes truncated when printed in the log file but the full name or expression is always given somewhere in the log file. The only limitations now should be on the length of file paths (260 characters as defined for non-Unicode versions of Windows) and the length of strings which are plotted. This remains at a maximum of 200 characters (Postscript imposes a limit of 255 characters for the maximum line length so very long strings are not possible anyway).

- A new input file parser has been written, partly to cope with the above. Please report any problems parsing or executing existing files. All functionality should have been retained, except as detailed below.
- In earlier versions of PhreePlot, a line following a line continuation character (`\`) was left justified before concatenating to allow for any indentation. Now there is no justification - where there is indentation, the extra leading space introduced is only likely to affect text strings that are plotted and which have been broken into two or more lines.
- A comment character (`#`) now takes precedence over a line ending character (`;`) and a continuation character (`\`) so

```
# line 1; line 2
```

will comment out both lines. This is consistent with PHREEQC input. Previously, a `#` only applied to the logical line on which it was placed, i.e. it would have only commented out line 1.

- A blank (or comment) line without a line continuation (`\`) character means that any existing line continuation is ended (`AsVsorptionvsph.ppi` adjusted accordingly), e.g.

```
plotTitle "This \
```

```
# a comment line
```

```
is the plot title"
```

would now produce an error.

- The diameter of the track symbol (a filled circle), that is for example used to show label anchors in custom plots, now accurately reflects `trackSymbolSize`. Previously like many other symbols, this symbol included an outer boundary space which meant that the actual diameter of the circle was only about 2/3 the specified symbol size. The default `trackSymbolSize` in `pp.set` has therefore been reduced from 1.5 mm to 1.0 mm to compensate.
- The `.inc` scripts for generating species distribution have been modified to take account of reported zero concentrations. This fixed a problem with occasional log species concentration plots, not just potentially trying to log zero but also out-of-order species data due to the lack of a placeholder.
- Tags can now be placed anywhere in an input file, not just in the Chemistry section. Character tag expressions can themselves be lists which are substituted as lists of numeric or character values in PhreePlot keyword definitions. This allows, for example, the list of plotted lines and points to be automatically generated. See the new example `demo\generatespecies\generatespecies.ppi`.
- Updated the documentation for the use of the latest versions of Ghostscript. However, Version 8.64 is still recommended.
- Minor bug fixes and changes.

- PHREEQC is now version 2.18.3-5570.

20 June 2011

Version 1

- Added a 64-bit version. This seems to run a little faster and can access more memory if available.
- A couple of minor changes.

16 June 2011

Version 1

- Release of PhreePlot Version 1.
- Development notes for the beta version have been archived on the Phreeplot website.