

## p:IGI+ release notes

### 3.0.1 (from 2.5.0)

Version 3 is a large update. We have increased the major version number as there is a significant change to the way the tools work with sites and boreholes (previously wells), which means that version 3.x of p:IGI+ will not be compatible with version 2.x of p:IGI+ or Metis. This is an important consideration meaning we will need to update both Metis and p:IGI+ at roughly the same time. We will be supporting clients using Metis for this update. We are also producing 'How-to guides' on the updated online user guide, to explain how to optimally update your v2.5 projects – see here: <https://userguide.igilt.com/software>.

### New/Improved features (p:IGI+ and Metis Transform)

- The concept of sites and boreholes (previously wells and non-wells) has been introduced to p:IGI+ and Metis
  - a site is a location shared by one or more samples
  - a borehole belongs to a site and represents a drilled shaft into the ground. It can be a common source of one or more samples. A site can have multiple boreholes associated with it.
  - Sites are merged by default on import to p:IGI+ based on (latitude, longitude), (or x, y coordinates), site name and location.
    - Transform will not merge sites automatically, this being done manually in the project merge and/or site/borehole merge
  - In p:IGI+ boreholes (which replace wells) are merged by default on import using the site, and the Borehole Name, UWI or Internal#.
    - Transform will not merge boreholes, this being done manually in the project merge
  - site properties can be harmonised, as can borehole properties (with the exception of the borehole name).
  - a new sites and boreholes manager sits below the artefact manager and shows the sites and boreholes in a project
    - this tree can be independently searched to find the sites and boreholes you want with the ability to show only sites, only boreholes or both
    - only when you apply a site or borehole to a visual artefact, like a graph, map or page is a site or borehole special 'static' sample set artefact created grouping those samples that are part of that site or borehole
      - when converting projects from v2.5 a set of borehole sample set artefacts will be created automatically
    - the site/borehole manager can be resized as desired to use as much or little vertical space as needed
    - the sites and boreholes respect the project sample filter, and will only be shown if at least one sample from them is included in the sample set applied
  - samples can be assigned to boreholes or sites from a right click on pages
    - a sample assigned to a borehole is automatically 'assigned' to the associated site

- a dedicated site and borehole editor has been created, available from the edit icon in the top right of the site and borehole manager
  - only one instance of the site and borehole editor can be opened at a time
  - the site and borehole editor can be configured to show any combination of site and borehole properties from a right click option on the headers
    - the layout is similar to a page, but in this case a row represents a site, or a site and its borehole
      - where a site has multiple boreholes the site data is repeated – editing one value updates all
    - columns can be frozen to the left, and unfrozen (similar to key columns, but only applies to the site/borehole editor)
    - users can sort on a selected column or revert to the default sort which is by Name.Site then Name.Borehole using a natural sort order
    - units of measure and display precision can be customised by the user and are remembered in the settings
    - counts are provided for each column – these represent the number of sites / boreholes with data
      - for sites this does not count ‘duplicated’ values across multiple boreholes at the same site
    - the harmonise option is available from right click on the column header
    - property help is available from right click on the column header
    - an individual property can be removed from the editor using a right click on the column header
  - all data can be edited in the page
  - copy will copy what is shown in the view
  - paste can be used for cells, or blocks – care must be taken to ensure the correct cells are being targeted
    - validation prevents pasting of incompatible values (e.g. strings in numeric properties) and errors are highlighted to the user, however any valid values will be stored
    - pasting a single value into a range will fill that range with the value
    - when pasting different values for the same site (where this has multiple boreholes, so appears multiple times) the final value is retained
    - undo/redo is possible using Ctrl+Z / Y or the Edit menu items
    - the Delete key clears the selected cells / values
  - you can create new sites and boreholes from a right click on the grid of the site and borehole editor
    - this can also be accessed from the Data menu
  - you can brush (and unbrush) sites and boreholes from the editor using the right click option – this selects (or deselects) all samples associated with the site / borehole

- any site or borehole with at least one sample brushed will show as being brushed using the brushing colour in the row headers
- Merge has been dramatically improved, allowing the user to explore more complex merges with feedback
  - merge now works in detail and respects the project sample filter – it is important that in large projects over 5,000 samples you merge in chunks to ensure performance remains acceptable
  - project merge now works over 3 stages: site merge, borehole merge and sample merge
    - sample merge can be run independently, skipping the site and borehole merge stages
    - site merge can be run independently to only merge sites
  - merge provides a detailed summary breakdown of the issues found when trying to bring together multiple rows of data
  - all data can be reviewed prior to merging, or the user can select to focus on only conflicts, or samples with missing merge criteria
  - the user can manually resolve merge conflicts
    - options are provided to automatically resolve conflicts due to precision differences, time difference and to prefer the most common value
      - these should be used with care as they can change data
    - the user can select to create samples sets and pages – merge diagnostics – to explore the merge on pages
  - the user can select a sample set to restrict the merge to a subset of data, and merge respects the project sample filter as mentioned above (to reiterate we encourage users to chunk the merge in large projects over 5000 samples)
  - it is now possible to merge samples not assigned to boreholes and sites with the samples which are assigned to boreholes or sites
    - this means **if you have good merge criteria**, for example unique sample names, you can import new analysis data for existing samples without having to attached borehole information and still merge with existing samples assigned to boreholes
- Collocation has been updated to include sites, meaning only samples at the same site or borehole will be considered as candidates for collocation
- Artefacts such as sample sets and palettes applied to other artefacts can now be removed from the top toolbar using a right click on the icon and selecting Remove
- Histograms can now be shown as stacked, overlain (most effective with transparency) or side by side to allow improved comparison of different populations
- Pages are more flexible
  - sort is now based on natural sort order so numbers in text properties are more naturally sorted, which is especially useful when sorting on borehole names for example
  - a palette can be applied to a page – this will colour the row headers using the palette colour, add a key to the bottom of the page window and allow you to filter samples using the palette
- Open artefacts are closed if the user selects to dock them in the workspace

- You can create the complement of a static sample set – that is a static sample set of all samples except the ones selected / in the static sample set
  - this can be done from the creation dialogue (without creating the sample set from the selected samples)
  - or from a right click menu on an existing static sample set
- The property selector, used across the system, will try and retain the indicators, units and ratios when a property is changed, rather than resetting these to the default
- A data QC tool has been added to run after import to populate missing data in a project, such as missing datums, site names or location information
  - the tool includes some basic QC rules including optionally creating sample sets for any samples where the top depth is below the base depth, samples that are below the associated borehole terminating depth and samples that report a depth but are not assigned to a borehole
  - the user can define their default preferences for the QC rules applied on running
  - this tool can be run on demand from the Data menu as well as after import, which can address issues caused when a user pastes data into a project, for example setting the depth datums so depth plots work as expected
- Time series plot axis labelling is more compact and natural
- Maps can have grids added in a range of formats (GeoTiff, NetCDF, ASCII grid, ESRI grid, ZMAP, Surfer .grd and Geopackage)
  - the grids must include projection information and will be reprojected into web Mercator for display on the maps
  - the user can select a continuous colour bar for the grid and define the range of that colour bar, which is shown nicely on the map legend
- Data from maps can be exported to shapefiles which creates a point layer as shown on the map
  - for numeric properties all statistics (mean, median, std dev, etc) from colour and size palettes are added to the associated database file
  - for discrete (text) properties, counts of each value are added to points in the associated database file, which can be used in e.g. QGIS or ArcGIS to create piecharts as p:IGI+ does
- A Geospatial data tool has been added to the Map menu to allow users to convert (X, Y) coordinates to (Lat, Long) coordinates
  - this will use the projections specified for each sample where they are valid, but will require additional information from the user where they are not set
    - this allows the user to convert from most widely supported local spatial reference systems
      - users can search for a projection using an epsg code where know this, or using descriptive text
  - this tool can be applied to a subset of the project using sample sets

## Machine learning features

Version 3.0 is the first release to enable the machine learning tools for all users. A basic version will be available to all users which supports the functionality to undertake: outlier detection, dimension

reduction using PCA, k-means and hierarchical clustering, linear regression and logistic (linear) classification modelling, and spatial interpolation on maps using inverse distance methods.

Advanced methods are available to all machine learning partners including soft cluster, various advanced regression and classification methods (neural networks, support vector machines, random forests, gradient boosting methods and probabilistic Gaussian process methods), improved spatial interpolation options including Kriging like methods (Gaussian processes), and a novel Bayesian unmixing tool which can be used for production allocation and general challenges around unmixing of mixed signals. All users have the option to subscribe to the advanced ML tools if they wish.

- A Bayesian unmixing tool has been developed
  - users can select the data set (samples and properties) they wish to consider for unmixing using a page and sample set
    - current system targets the use of concentration measurements (must be positive, with assumed log-Normal proportional error distribution) and unconstrained properties (can be negative and positive, with assumed Normal or Gaussian error distribution)
    - users can define the errors on the properties
  - users can provide end members, or use the automatic Vertex Component Analysis (VCA) methods to identify candidate end members
    - brushing can be used from the project to define the end members
  - users can specify their confidence (their prior in a Bayesian setting) over the end members, either individually or for all end members
  - the algorithm finds the maximum a posteriori probability end members and mixing weights using a novel algorithm inspired by alternating least squares methods
    - mixing weights (proportions) are returned to p:IGI+ for each sample sent
    - the identified end members can be exported to an Excel file (with the mixing weights and other model information) – these can be imported back into p:IGI+ if needed
  - full interactivity is provided including univariate outlier removal, missing data treatment, and model initialisation
- Spatial interpolation has been added as a right click option on the map
  - will interpolate the continuous valued property selected based on the colour palette by default
    - use a sample set to limit, e.g. to a given formation
  - provides the option to transform the interpolation target based on its distribution – option for log and square-root transformations are especially useful for positive properties
  - user can add a grid to provide additional information, e.g. a depth grid or other ancillary information
    - this is used with spatial location to improve the interpolation
  - simple inverse distance method provided as a baseline, but full tool includes trend surface analysis, spline and Gaussian process (Kriging / geostatistical) models
  - diagnostics are provided on the quality of the interpolation, similar to regression models

- tool provides control over the prediction grid size and how far to extrapolate beyond the observations
  - grid can be saved as a geotiff format which can easily be applied (using drag and drop) to any map in p:IGI+, but can also be imported to all GIS systems
- A semi-automated machine learning model selection option has been added allowing you to explore a range of model choices quickly and easily
  - the user can select a model of their choice from the trained options, with the 'best performing' automatically suggested
  - we have added a 'gridsearch' engine to make this process fast for the user, by spinning up enhanced compute capability
- Novelty detection has been added to the ML pipeline providing the user information about how different the data on which the model was trained is from the data being used in predictions
  - this will help alert users to the case of the model being over-confident on data it has not seen before – a novelty score is returned which can be shown alongside the predictions
- The machine learning tool window is no longer modal, meaning you can still interact with p:IGI+, for example to explore specific samples in greater detail, while training the ML models
  - this means we have been able to add support from brushing to and from the ML tools, with almost immediate synchronization with p:IGI+
  - we have implemented support for brushing in almost all the ML tools including in the 3D and 2D plots and regression diagnostics, although support will be further improved in maps (spatial interpolation) moving forward
- ML model predictions can be used as inputs to project properties, although care should still be taken when doing this to avoid chains of inputs, or issues if a model is renamed
- The display of many of the diagnostic plots has been moved to the front end (making them more interactive)
  - the ROC plot now allows you to vary the decision threshold to help understand the meaning of the curves
- Outlier detection uses a robust scaler to minimise the challenge of working with data which contains extreme values
  - we also provide the option to use elliptic envelope outlier detection as well as the isolation forest option
- Value outliers that represent potentially erroneous data can be discovered at the tool startup to remove their effects from further exploration
  - the user is presented with a default sensitivity and preview dot-plots which enables them to tune the value outlier sensitivity choice
  - the user is provided with the option to set a per property sensitivity if wanted
  - value outliers are removed from the data and treated as missing values
- We have improved the retraining of models, although this does result in a slightly longer time to save the model to p:IGI+
  - the retraining now first provides a view onto the trained model, then allows the user to start from identical settings and being to explore changing those and training again

- The “Find a good data set” tool has been improved to make it easier to provide precise values for the sliders supporting easier reproducibility

## Metis features

- The concept of sites has been introduced to Metis
  - a site is a location shared by one or more samples
  - sites have their name populated according to the common-prefix of their associated borehole names
  - we have added a sites tab to Metis Discover and Transform Online
  - sites and boreholes can have their metadata updated in Transform Online in the newly added site manager
  - sites and boreholes can be deleted from within site manager
    - Deleting all the boreholes and/or samples will also delete the associated site
  - in Transform, uploading data to staging has an additional site stage where matching sites in Metis are identified and conflicts can be resolved
- Stratigraphy (tops and trajectories) can now be bulked uploaded via Transform Online
  - using an excel template chronostrat and/or lithostrat can be uploaded to multiple boreholes and assigned to either primary or alternative stratigraphy
  - differences in the uploaded stratigraphy are reported and a data manager can choose to update when
  - stratigraphy is then assigned to samples accordingly
  - a borehole’s stratigraphy can be viewed in the site manager
  - stratigraphy is downloaded from Metis into p:IGI+ when linking data
  - stratigraphy from Metis can also be updated within p:IGI+ separately
- p:IGI+ v3.0 can link and download data from Metis v3.0 (and above). However, Metis v3.0 is not compatible with earlier versions of p:IGI+
- The Metis tab in the settings menu has been improved:
  - expired sessions are detected so only Metis environments where login details are still valid are shown
  - environments can now be removed from the Metis settings dialogue in p:IGI+ and Transform

## Property model

- To accompany the introduction of a new approach to handling location information (see new and improved features section above where wells & non-wells have been replaced with sites & boreholes), the following edits and additions to the property model have been made:
  - the previous **.Well** property group has been renamed to **.Site** and a **.Borehole** group has been added.
    - The site group contains details on the site name/description, site position and site geographic/geologic location, absolute datum and site elevation/depths
    - boreholes contain details on the borehole name/description, drilling information, bottomhole information and depth datums of the borehole

- the existing **.Sample** property group remains, but the geographic properties for the previous “non-well locations” have been removed, with data merged into appropriate **.Site** group properties
    - two properties, Location.Sample, and Campaign.Sample remain that can be used at the sample level, but we advise using the **Location.Site**, and **Campaign.Site** properties, as Metis only supports the site variants. This is especially important in Metis Transform
  - An automatic migration of existing project well/non-well location/metadata will take place when version 2 files are opened in V3.0. It is advised that users should run a site-level merge and the Data QC tool to ensure correct site groupings and link creation between sites and boreholes.
- The (**Visk-RL**) group has been reviewed, and work completed to incorporate new maceral properties and aliases. This will assist with linking during import and will see more data being stored.
    - Exsudatinite (**Exsu**) has been added to the Liptinite scheme, and the hierarchy equations have been updated accordingly.
    - Gelinite (**Gel**) and Corpogelinite (**Corp-gel**) have both been added to the Vitrinite scheme and the hierarchy equations updated accordingly.
    - Secretinite (**Sec**) has been added to the Inertinite scheme, and the hierarchy equations have been updated accordingly.
    - Sclerotinite (**Scl**) has been renamed to Funginite (**Fung**) to match the more commonly used term for fungal remains.
      - *Sclerotinite was previously used to describe both fungal remains and certain oxidised plant secretions; the term is now obsolete, with these components now classified as funginite (fungal remains) and secretinite (oxidised plant secretions), (O’Keefe et al., 2013).*
  - Discussions with clients and analytical vendors have led to improvements in the **Py-GC** and **Py-GC-Extr** property groups.
    - descriptions updated for the total resolved fraction properties to indicate that the input values to the existing Primary (APT used) Py-GC scheme (C1, C2-5, C6-14, C15+, GasFract, OilFract, GOGI) should be inclusive of the UCM.
    - a new set of total resolved fraction properties has been added to allow the loading of data exclusive of the UCM have been added (C1xUCM, C2-5xUCM, C6-14xUCM, C15+xUCM, GasFractxUCM, OilFractxUCM, GOGIxUCM).
    - in order to appropriately create and plot data on the 1989 Horsfield chain-length distribution ternary plot, the C6-C14 and C15+ properties require only the n-alkanes and n-alk-1-enes. Consequently, two new properties with a sum equation have been added to create appropriate axis properties: AlkSumC6-14 and AlkSumC15+
    - sample weight (Sam wt) added to the **Py-GC** and **Py-GC-Extr** groups
    - updated Geochem help descriptions for the Py-GC and Py-GC-Extr properties to reference them to the pyrolysis production gas chromatography analytical method that is run

- Across all **Gas** and **MudGas** groups, we have edited the following gas ratio properties to ensure the presence of an [\*]any indicator, appropriate target units, ratio format, etc.
  - He/Ne
  - C1/N2
- New **Gas-Iso** ratios have been added to the property model:
  - d13C nC4-iC4
  - d13C C1-C2
  - d13C C1-C3
- A series of short-chain A-ring methylated steroidal hydrocarbons from the m/z 231 and m/z 245 have been added to the **Sat-GCMS** and **Arom-GCMS** group. Along with the property ratios, properties with associated equations have been added to plot age-determining plots published in Killops et al. (2023)
- The Terrigenous-Aquatic Ratio (TAR),  $(nC27 + nC29 + nC31) / (nC15 + nC17 + nC19)$ , has been added to the **Sat-GC**, **WO-GC**, **HT-GC** and **TE-GC**
- A series of VR maturity equivalence properties have been added to the property model
  - %R(iC4/nC4) – taken from Arouri, (2024)
  - %R(iC5/nC5) – taken from Arouri, (2024)
  - %R(Ts/Tm) NO – taken from a published report from DISKOS
  - %R(Ts/Tm) Bennett – taken from Bennett & Larter, Geoconvention, Calgary, Canada (2019)
- The parameters Methcyclohexane Index (MCyC6Index), Cyclohexane index (CyC6Index) and Sum dimethylcyclopentane (SumDMCyC5) have been added to the **Gasol-GC**, **TE-GC**, **WO-GC**, **WO-GCMS**, **MudGas**, **MudGas-Corr**, to assist in identifying the source origin of thermogenic gas. The sum of the dimethylcyclopentane property enables the source-based triangular plot from Huang et al., 2025, to be created
- A series of existing GCMS saturate ratios have been created in the **GCMS-MS** and **MRM-GCMS** groups
  - H33 22S/R , H34 22S/R, H35 22S/R
  - H30ab/H29ab
  - Dia29/St29aa
- Ratios have been added to a range of **WO-GCMS**, **Sat-GCMS**, **Arom-GCMS**, **Diam-GCMS**, **GCMS-MS**, **MRM-GCMS** properties. The majority of properties were methylated diamonoids
- New property groups were created to accommodate the loading and storage of Rock-Eval 7/7S (**Pyol7S** & **Pyrol7S-Extr**), both pre- and post-extract. The majority of the properties were duplicated from the Pyol6 and Pyrol6-Extr groups as the same core functionality is present across both machines. The additional capabilities of the Rock-Eval-7S is when it is used to measure and determine the presence of organic, mineral and total sulfur in rock, kerogen, coal, shale, oil (reservoir) samples. New properties, Sum properties and Ratio properties, have been created for the peaks derived from the SO2 detector measuring sulfur products formed during the pyrolysis and oxidation cycles
  - the TOC. Any properties will be updated to include RE7 TOC in the following release
- Lithium, Ferrous Iron and Ferric Iron elements have been added to both the **XRF** and **Inorg** groups. The ratio Zr/10 will also be added to both groups to enable elemental provenance and palaeotectonic setting triplots to be created

- Properties associated with water samples have seen several additions and edits.
  - A range of commonly reported BTEX and Organic acids have been added to the **Ions** group
  - New unit conversions between mol/vol, wt/vol, and meq/vol have been added for the **Ions** group properties
    - With meq/vol units present, then standard hydrology plots will become possible to create / display data
  - Property descriptions for Ions group properties have been updated to specify the ion charge to ensure users are aware of what data is correct to link to ensure the new unit conversions are accurate
- A full review and update of the Geochem Help information and property code lists/alias lists linked to the new/edited property groups has been completed

## Fixes

- When changing the search term in the property selector we now always return to the top entry to ensure the user sees the most relevant suggestions
- When a lot of graphs are open at the same time, or after long use of p:IGI+ sometimes you get no points shown on a graph, and a text error message saying "E\_OUTOFMEMORY: Ran out of memory (\*\*\*)". To address this save the project, close p:IGI+, restart, and open the project. We have fixed this issue with the upgrade to support the latest .NET version
- Occasionally when resizing graph windows the data view can pan unexpectedly. This is a rare event, but has now been fixed
- When a user loses connection to the licence server p:IGI+ will now behave more gracefully, allowing the user to save their work and exit
- Fixed a potential security vulnerability in auto-artefacts
- Dates prior to 31<sup>st</sup> December 1899 are now exported correctly, addressing an Excel limitation
- Cloning a statistics artefact will now produce an identical copy of the original artefact
- Sample counts on the top of pages are now correct for project properties with the [\*] any indicator
- Editing a project property equation used to not update properly when adding a new exists{} clause – this has been fixed
- Property help will now correctly jump to provide help on a property selected from a page even if the property help is already open
- Addressed some issues when creating and editing overlay / underlay objects in the overlay editor.

## Known issues

- From version 2.5 onwards p:IGI+ will no longer open version 1.x projects. Older projects should be converted to version 2.0 or later before updating to 2.5 or later. IGI will be able to provide a tool or a service to update old projects if needed.
  - p:IGI+ version 3.0 will migrate projects to the new .pigi3 format – these will not be able to be opened in p:IGI+ 2.x

- The “Sitka” font family does not work when copying graphs – it displays fine, but the graphs will not copy correctly. We advise users to not use this font family, which has some known issues in Windows
- The Excel import template for site/borehole data (Project --> Import site/borehole data...) only allows the import of metadata when a valid borehole name is present (Name.Borehole). The import of site only metadata is currently not possible.
- Following the addition of the Pyrol7S and Pyrol7S-Extr property groups the associated TOC properties have not been added to the TOC.Any, TOC\_Bulk.Any and TOC\_Extr.Any properties.

## Installation issues

Requires .NET framework version 8.0