Petrological Input Graphical oUput (PINGU): an online tool for plotting geochemical diagrams.

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Abstract

In this contribution we introduce PINGU 1.6 (**P**etrological **IN**put, **G**raphical o**U**tput); an online tool to generate plots commonly used in igneous petrology & volcanology, based on whole-rock, major and trace elements geochemical data. The output generated by PINGU are a high-quality, publication-standard JPEG or an EPS files, which can be used in professional papers or in the classroom at undergraduate or graduate level, in the context of teaching igneous petrology or volcanology. Some of the current diagrams available in PINGU 1.6 (new diagrams are implemented on a regular basis) are the total-alkali vs SiO_2 diagram, the K_2O vs SiO_2 diagram, ternary diagrams, the REE diagram or the spider diagrams. The tool is a multi-platform online resource and freely available in Vhub (*http://vhub.org*), a cyberinfrastructure for the volcanological community.

Keywords: cyberinfrastructure, Vhub, Work-flow, Geochemical Diagrams, Petrology

1. Introduction

Geochemical data sets are multivariate and usually large, therefore the natural necessity for their graphical representation for visualization (Rollinson, 1993). In particular, in the fields of igneous petrology and volcanology, such necessity has produced a vast collection of diagrams, which are typically used for classification or interpretation of the geochemical data sets. However, there are difficulties associated with highly specific plots, because standard plotting software is inadequate (particularly for some highly-complex diagrams), produce low-quality outputs, it is platform-specific or it is simply out of date. Most standard diagrams based on geochemical data are used for classification purposes, the discrimination of tectonic settings or for testing petrogenetical models. The following is a list of examples of diagrams used in these three categories:

i) *Diagrams used for classification purposes.* For example, the Total alkali vs. Silica diagram (Le Maitre et al., 1989) or Nb/Y vs Zr/TiO_2 (Winchester and Floyd, 1977). These plots are usually bi-variate and the different classification fields are divided by empirical lines.

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ii) *Process-related and interpretative diagrams.* A typical example are the so-called Harker (1909) variation diagrams (major elements vs SiO_2 in wt%), which are normally used to infer the evolution of magmas due to fractional crystallization and/or magma mixing in a genetically-related suite of chemical analyses. In a sample suite it is possible to calculate from direct inspection in these diagrams the proportion of the fractionating mineral phases by means of the lever rule (e.g. Cortés, 2009). Usually these plots do not have specific fields, but sometimes they require a specific range or scaling of the axes. For example, variation diagrams in which MgO is in abscissa, require the abscissa reversed, or, in the case of lever rule calculations, the variables must be plotted using the same scaling.

iii) *Tectonic-Setting-related diagrams.* These are diagrams based on fully empirical correlations in the data, in which the plotted fields represent a given tectonic setting (e.g. Pearce, 1983; Pearce et al., 1984). These diagrams can be simple to generate (e.g. Pearce et al., 1984), although the plotting fields are sometimes difficult to reproduce.

In this contribution we introduce "**P**etrological **IN**put **G**raphical o**U**tput" (PINGU); an on-line multi-platform tool that provides many of the three types of diagrams, with high quality rendering of the plots in the Joint Photographic Experts Group (JPEG) and Encapsulated Postscript (EPS) formats. The tool can be freely accessed through Vhub (*https://vhub.org*), an online resource for collaboration in volcanology research and risk mitigation (Palma et al., 2014).

1.1. The Vhub cyberinfrastructure

We have chosen to implement PINGU as an online tool in the framework of the Vhub platform (*https://vhub.org/tools/pingu*). Vhub is a community cyberinfrastructure specifically dedicated to volcanology and hazard mitigation, currently funded by the US National Science Foundation (NSF) and sponsored by the International Association of Volcanology and Chemistry of the Earth's Interior (IAVCEI). Vhub fosters collaboration among researchers, students, volcano observatories and any individual working toward reducing volcanic risk (Palma et al., 2014). The community can discover and learn new information and knowledge through courses, workshops and individual presentations hosted online, as well as from blogs and technical wiki documents. Becoming a member of Vhub is free, fast and straightforward. Registered members of Vhub have a personalized dashboard for organizing their favorites resources, applications, groups that they have joined, a profile description and a personal blog. Vhub's resources are grouped into Courses, Data Sets/Collections, Educational Materials, Presentations, Publications, Workshops, Offline Tools, online Tools, and Miscellaneous. A detailed description of the Vhub infrastructure can be found in Palma et al. (2014) and in *https://vhub.org/about*.

Vhub hosts interactive applications in their own servers that can be run from any computer, provided that it is equipped with a fairly fast Internet connection and a standard web browser with an up-to-date JAVA Plug-in. An advantage of this implementation is that online tools are platform-independent, running on Linux, Mac and Windows machines. Software updates are carried out by the developers within the Vhub platform without the need of any user's interaction. Thus, PINGU is readily available to students and researchers needing to create high-quality plots from geochemical data sets. Within Vhub, each registered user has allocated 1Gb of storage space accessible through the Web Distributed Authoring and Versioning protocol "WebDAV", or through the online tool "Workspace", which resembles a Linux (Debian) terminal. Accessing the user's personal files is sometimes necessary in order to upload or download the results of some applications. The Workspace is also useful for developers willing to test and edit their tools in the Vhub platform.

Taking advantage of Vhub resources, we have also created the "PINGU Appreciation Society" (*https://vhub.org/groups/pingu*), an online resource in which manuals, examples of input data, discussion and support for PINGU are available. Prior to using PINGU, the user must join this group by simply clicking the "Join Group" button in the welcome page of the group (Figure 1). By joining this group the user has full access to manuals in wiki format (*https://vhub.org/groups/pingu/wiki*), which are actively updated, and examples of spreadsheets with input data in the correct format. The group also provides mechanisms for bug reports, questions and general support, as well as an option for requesting new features to be added in future implementations of the tool (Figure 1). For the authors, the group provides dedicated feedback from the users and a mechanism to provide timely support.

2. PINGU workflow

The implementation of PINGU 1.6 has been done as a computer work-flow including several components running in Vhub's Debian server:

- The Rappture toolkit (Rapid application infrastructure) (McLennan, 2005b,a), a basic infrastructure for the generation of graphical user interfaces (GUI) that can be linked to an underlying processing code. Based on a description of inputs and outputs, using the Extensible Markup Language (XML), Rappture generates a GUI and allows other programming languages such as Perl, Python, GNU Octave, C/C^{++} or JAVA, to access all the values in the input fields of the GUI. After processing the data, the code can send the results back to Rappture for displaying in the GUI.
- GNU Octave (Eaton et al., 2008), a MatLab-like scripting language (*http://www.gnu.org/software/octave/*). Octave offers great flexibility for reading and saving data, and for matrix operations.
- GNUPLOT (Janert, 2009), a widely available multiplatform plotting utility (*http://www.gnuplot.info/*). GNUPLOT allows the generation of high-quality plots from a source code.
- ImageMagick (Still, 2005), a free software suite to edit and convert bitmap images (*http://www.imagemagick.org/script/index.php*).

The Rappture GUI interface (Figure 2) pipes the user's data and selected options into GNU Octave, which processes the geochemical data and generates a file with a specific format for plotting. This file is available for further processing in the user's personal storage within Vhub. After processing, GNU Octave opens a pipe into GNUPLOT, which generates the figures. GNUPLOT produces an EPS version of each plot (and optionally the plot's Key, see below), saves it in the workspace and exits. GNU Octave then pipes the EPS image into ImageMagick, which converts it into a high-quality (density 300 dpi) JPEG image. GNU Octave finally pipes the JPEG image back into the Rappture interface, from which it can be directly downloaded through the web browser.

3. The application

After the user has joined Vhub and the Appreciation Society Group, the tool can be launched from *https://vhub.org/resources/pingu*. The web browser will open a JAVA applet window in

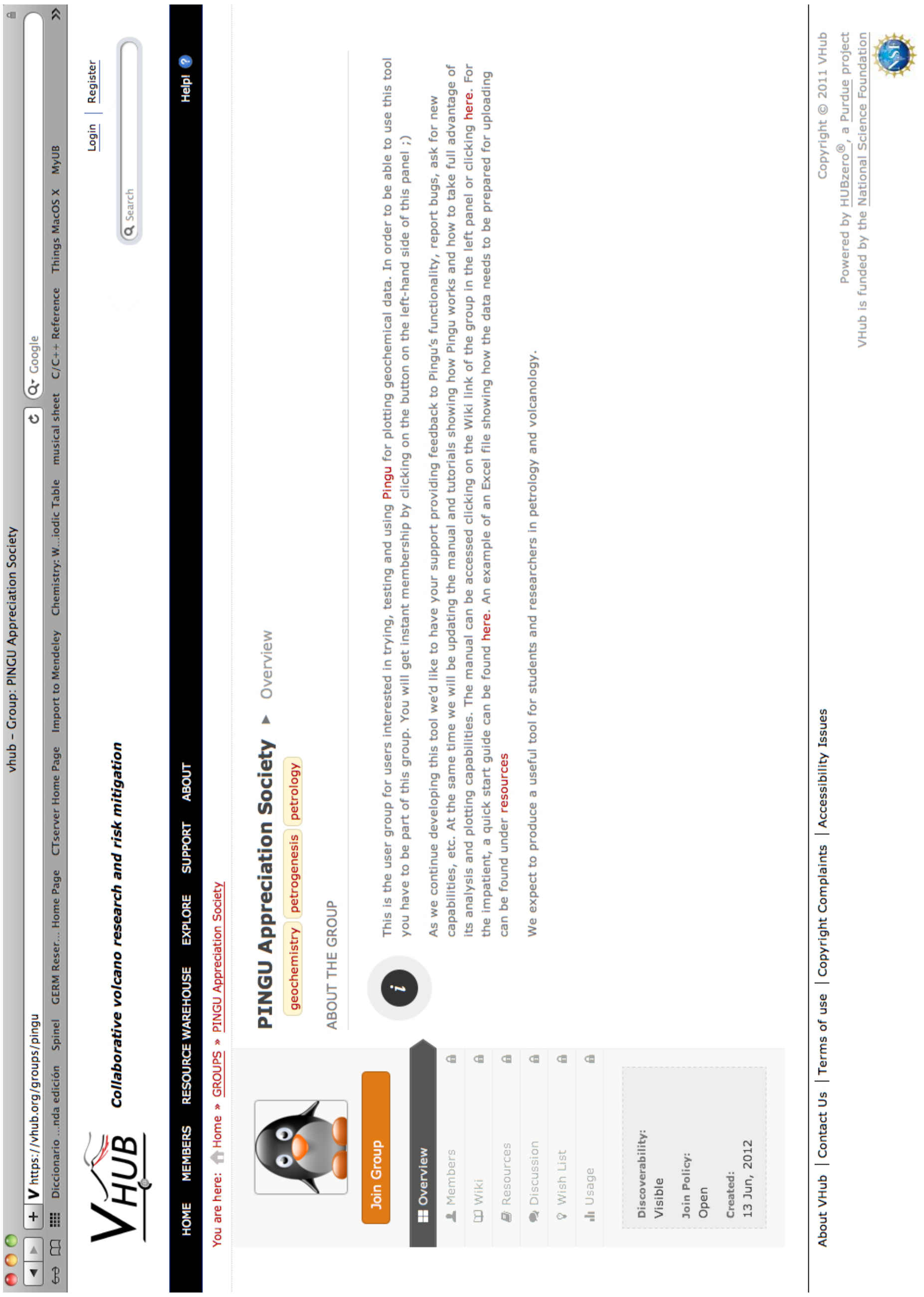


Figure 1: The welcome page for the PINGU Appreciation Society Group. Note the orange button prompting for joining the Group. The menu on the left-side of the page provides access to the wiki, resources, discussion and wish list for the tool.

which the GUI of the tool is presented (Figure 2). The data is uploaded into the input window from the “local machine” (i.e. uploaded directly from the user’s computer through the browser) or from the Workspace (i.e. from the user’s personal storage within Vhub).

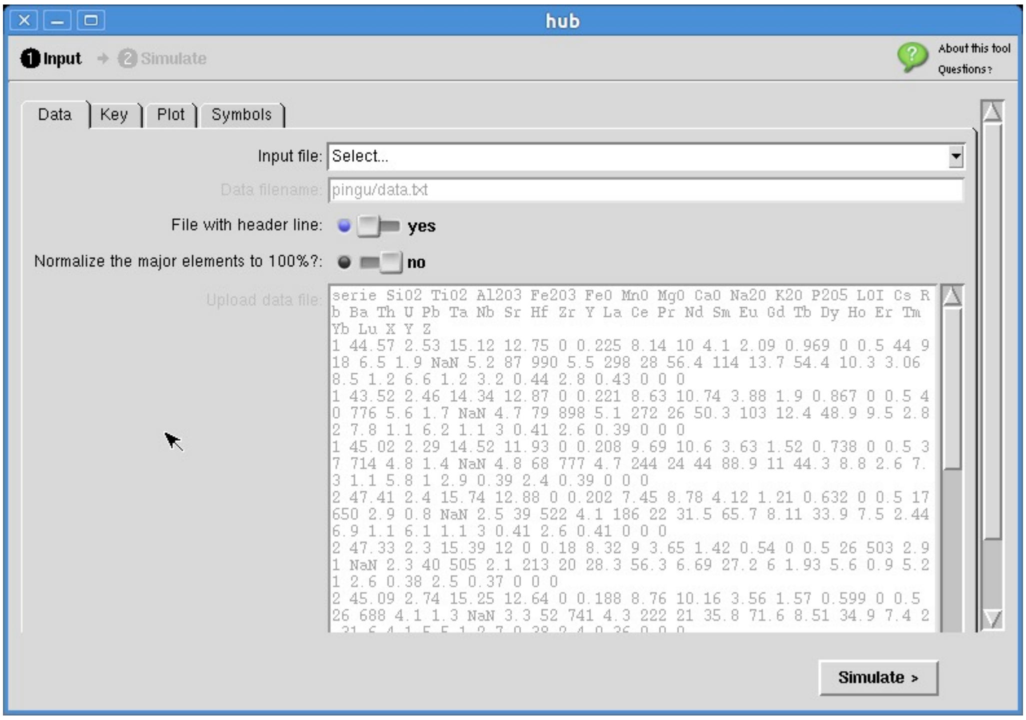


Figure 2: PINGU graphical interface (Linux version), showing the main window where the data is uploaded (Data) and the different tabs (Key, Plot, Symbols) in which the user can select the type of plot, Key (legend) and custom symbols. The main window also allows the user to select whether the data will be directly uploaded from a local machine or from Vhub’s workspace (“Input File” tab), whether the major elements should be normalized to 100% or whether the processed data will be saved in Vhub’ Workspace.

The specific plot, design of the key and symbols are selected clicking in the corresponding tab (Figures 3,4 and 5), although a specification of a key and customization of symbols are not required to generate a plot (in the first case the key is not produced, while in the second the plot is generated using PINGU’s default set of symbols).

3.1. Data Input

The data are uploaded directly from the user’s computer by selecting “local machine” in the “Input file” tab or from the user’s workspace in Vhub, selecting the “workspace” option. Right-click (PC, Linux) or Command-click (Mac) on the data window will upload the data from the “local machine”, while entering the path and name of the data file in the user’s workspace will upload the data from the user’s storage space in Vhub.

The data file has to be formatted as a text file (UTF-8) separated by spaces or tabs, with or without a heading line. This file can be prepared in a standard spreadsheet program. The data set should contain each data point in a row with the following columns: *“series”*, SiO_2, TiO_2,

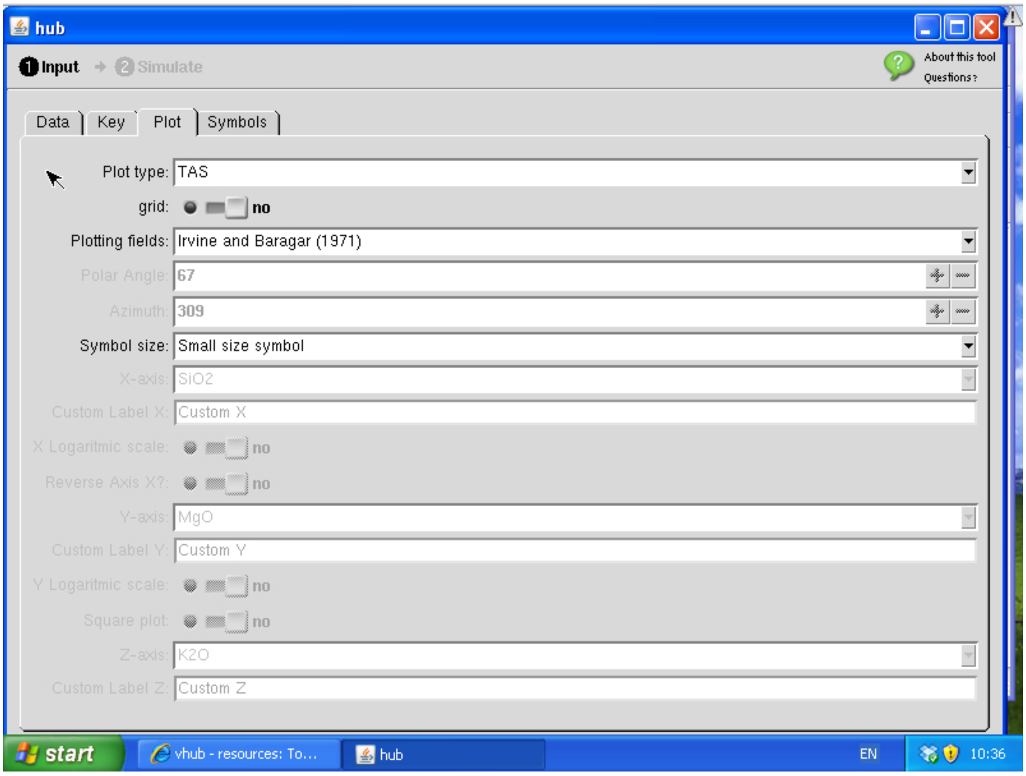


Figure 3: PINGU graphical interface, showing the Plotting Tab (Windows version). In this window the user can select the plot and customize it adding a grid, selecting the symbol size, logarithmic scale, reversed axes or same axis lengths.

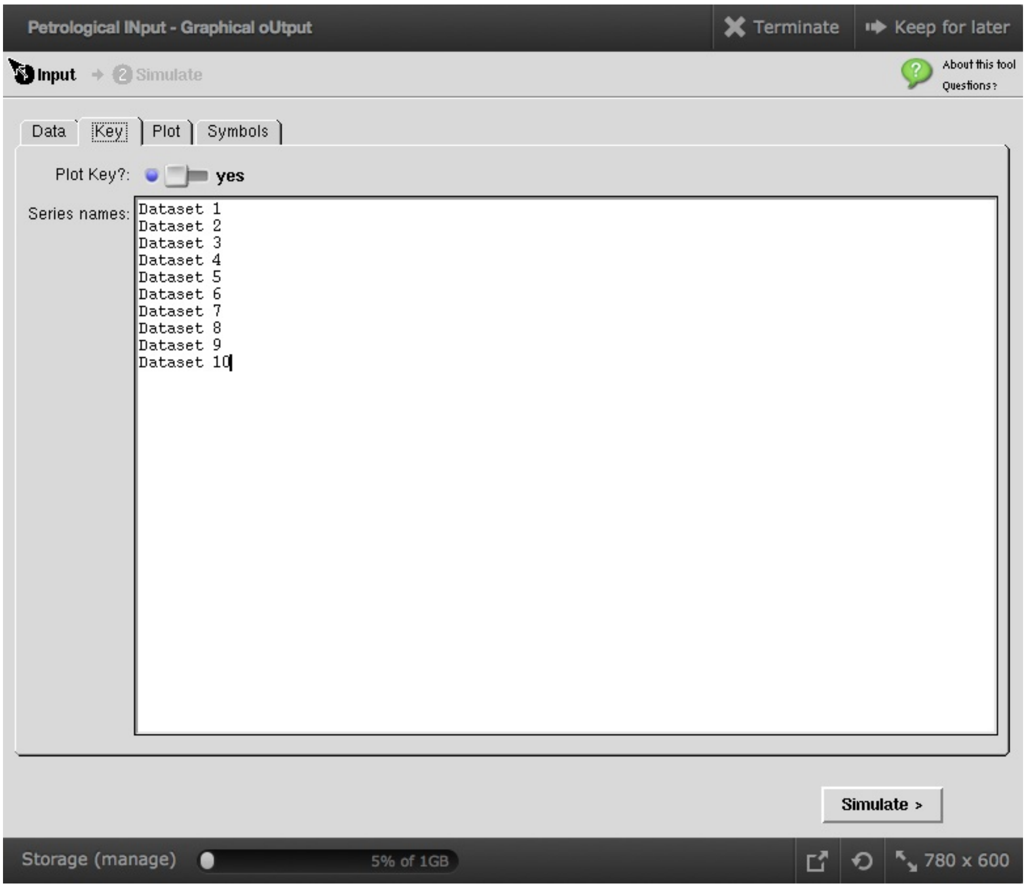


Figure 4: PINGU graphical interface showing the Key tab (Macintosh version). This menu is optional and can be activated selecting "Yes" under the "Plot Key?" label. When activated, the user can type the names of the different plotting units. When the plot is generated, the key is created as an EPS and a JPEG files with the name of the units and symbols used.

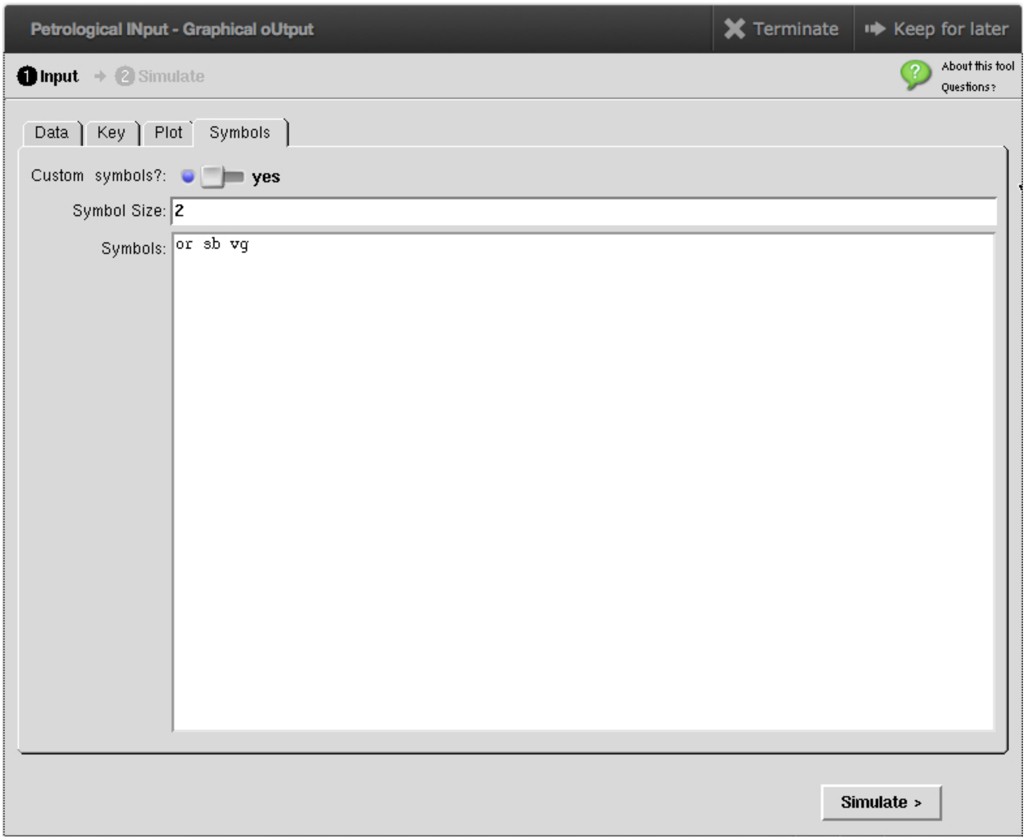


Figure 5: PINGU graphical interface, showing the Symbol tab (Macintosh version). This menu is optional and can be activated selecting "Yes" under the "Custom symbols?" label. When activated, the user can type, in a MatLab-style string, the custom symbol specification (in the example, the first series will be plotted with red circles, the second with blue squares and the third with green triangles) and the symbol size in points. If no custom symbols are selected, PINGU will generate a plot with its default set of symbols and colours.

Al_2O_3, Fe_2O_3, FeO, MnO, MgO, CaO, Na_2O, K_2O, P_2O_5, LOI, Cs, Rb, Ba, Th, U, Pb, Ta, Nb, Sr, Hf, Zr, Y, La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, *"custom X"*, *"custom Y"*, *"custom Z"*. The decimal separator for all values must be a dot and not a comma. An example of a spreadsheet with the correct format can be downloaded from the Resources of the group at *https://vhub.org/groups/pingu/resources*.

The first column ("series") should contain integer numbers that identify a group in the data to be plotted with a specific symbol. For example, if there are three different units to plot, the different samples in each group can be labelled 1, 2 and 3. There is no restriction on order or value of these numbers, providing that they are integers and each group has a unique value. To avoid a segmentation fault error, *all the cells of the input file must be filled*. If an element in the analysis is not known, then the associated cell should be filled with the string "NaN" (i.e. "not a number", without the quotation marks). In the particular case when the speciation of the iron is not known, the total iron can be uploaded either as $FeO^{\star}$ or $Fe_2O_3^{\star}$ filling the other column with "NaN". After the data is uploaded and displayed in the window, the user can opt for normalize the major element data to 100% or continue with the raw inputted data (Figure 2).

3.2. Key

As an optional feature, an independent key file (in JPEG and EPS format), can be generated at the same time when a plot is produced (Figure 4). Clicking in the "Key" tab and selecting "Yes" will activate a window in which a string for each series, consistent with the uploaded data, can be entered. If the number of strings is lower than the number of series given in the data set, PINGU will produce a key in which the symbols with no information will be plotted without a label. If more strings than series are provided, PINGU will simply ignore them.

3.3. Symbols

PINGU 1.6 have by default a hierarchy of symbols and colours, which, in the opinion of the authors, have a good rendering in both colour or Black & White outputs. However, if the user requires specific symbols and colours, these can be entered as string in the "Custom Symbols" window (Figure 5). The string must contain one character for the symbol and then another for a specific colour. The symbol scheme and colours follow loosely a MatLab style definition and are presented in Figure 6. For example "or +k vg" means that the first series' symbol will be a red open circle, the second a black cross and the third a green open upside-down triangle. If there are more symbol definitions than series, the extra symbols will be ignored. If there are less, the remaining series will be plotted with random symbols. PINGU version 1.6 currently allows a maximum of ten custom symbols. Additionally, the custom sizes of the symbols ("small", "medium", "large") can be modified if this option is selected, providing the option of inputing the symbol size in points (Figure 5).

3.4. Plotting

After a plot is selected scrolling the "Plot type" tab (Figure 3), the available options for that specific plot will become active (see below for more details on those options). Clicking on the "Simulate" button below will generate the plot and, if it has been requested previously, the key in the same Output window, either available by pressing the "Result" tab (Figure 7a,b).

Symbol	Character
⊡	s S
■	$
⊙	o O
●	0 (number zero)
◬	^
▲	A
▽	v V
▼	w W
◈	d
◆	D
◐	<
◑	>
+	+
×	x X
✳	*

Figure 6: Available set of symbols for custom plots in PINGU. Available colours are “b”, blue; “k” black; “r”, red; “y”, yellow; “g”, green; “m”, magenta. Note that some symbols can be generated with more than one type of character, however the inputted string only should contain only one of these.

3.5. Output

PINGU 1.6 typical output is the requested figure in JPEG format presented in the output window after selecting it from the "Result" tab (Figure 7a), which can be downloaded by clicking on the "green arrow" icon in the upper right of the window. Alternatively, the user can also request an EPS version of the plot using WebDAV, or the text file with the values used in a specific plot through their Vhub's workspace if that option has been previously selected. Selecting "Key" in the "Result" tab will display the key for the plot, which can be downloaded clicking the same " green arrow" icon (Figure 7b). Clicking on the "Input" label (in grey above) or the "< Input" button (below), will bring back the starting plotting window in which a new plot can be selected, using the same uploaded data set, the same user-defined key and custom symbols.

4. Available plots in PINGU 1.6

The following is a list of the current plots available in PINGU version 1.6, which can be accessed through the "Plot Type" tab in the Plot Window (Figure 3). Depending of the plot selected, some additional options may be available. Users can request the implementation of new types of plots through the "PINGU Appreciation Society" under the "Which list" tab (Figure 1).

i) Variation diagrams versus SiO_2 (Harker, 1909), which are presented in a single figure. If a single variation diagram is needed, it can be plotted as a "custom plot" (below). The diagram can be produced with or without grid and custom symbols, however the symbol size cannot be changed.

ii) Variation diagrams versus MgO, also presented as a single figure. As usual, these diagrams show MgO in the abscissa with reverse values. Available options are the same than for Harker (1909) diagrams.

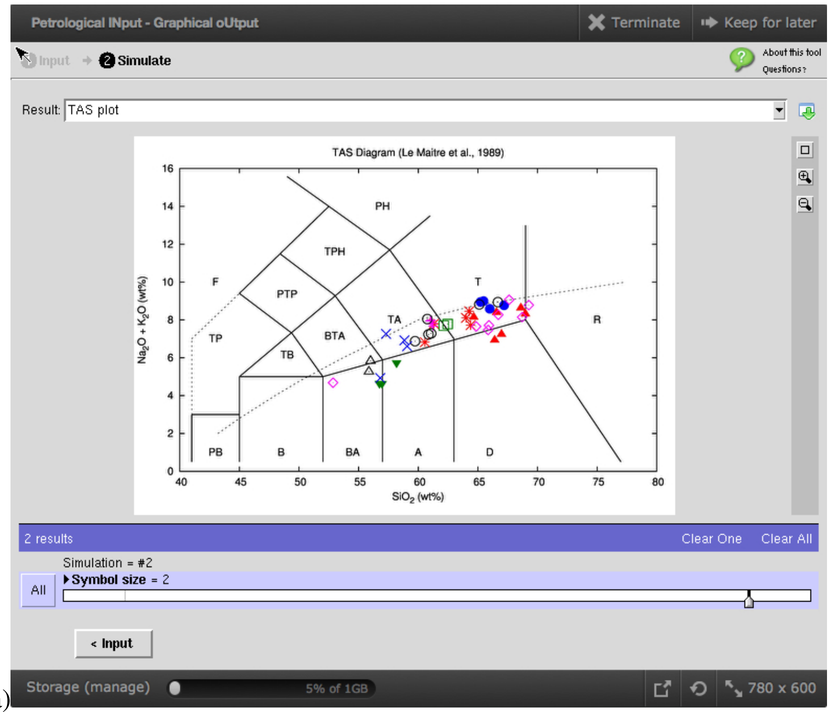
iii) Total alkali versus Silica ("TAS" diagram). The official IUGS classification diagram for aphanitic rocks introduced by Cox et al. (1979) and modified by (Le Maitre et al., 1989). The diagram can be rendered with or without grid, with or without the alkaline/sub-alkaline boundary of Kuno (1968) or Irvine and Baragar (1971), custom symbols and three different symbol sizes (Figure 7a).

iv) Total alkali versus Silica ("TAS" diagram), in its original version proposed by Cox et al. (1979) and the modified version for igneous rocks introduced by Wilson (1989) The diagram can be rendered with or without grid, with or without the alkaline/sub-alkaline boundary of Kuno (1968) or Irvine and Baragar (1971), custom symbols and three different symbol sizes (Figure 7a).

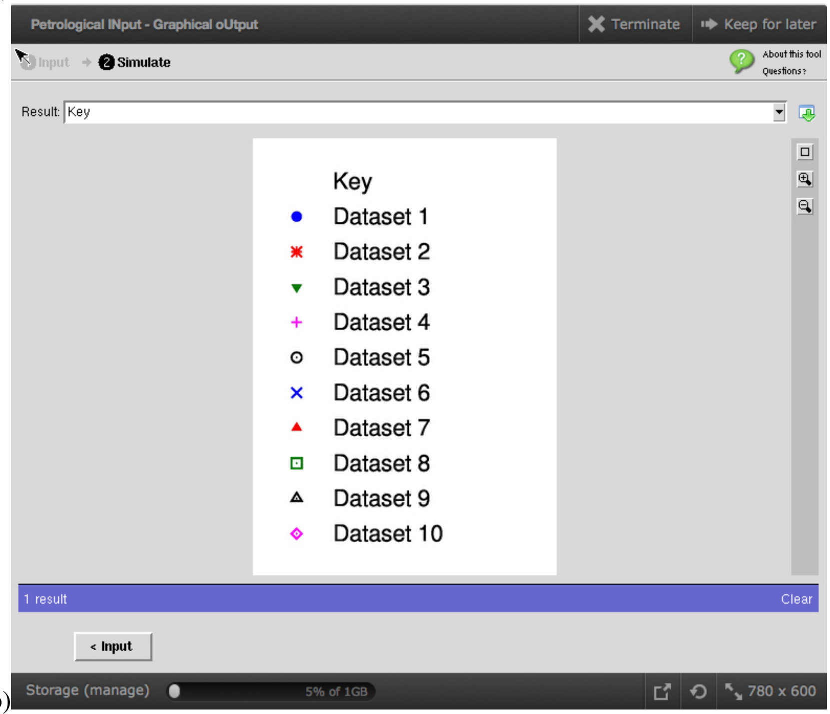
v) The K_2O vs. SiO_2 variation diagram as a classification diagram. PINGU produces this diagram with the boundaries proposed by Peccerillo and Taylor (1976); Ewart (1982); Innocenti et al. (1982); Carr (1985); Middlemost (1985) summarized as bands in Rickwood (1989). Vertical lines were compiled from Winter (2010). The diagram can be rendered with or without grid, custom symbols and three different symbol sizes.

vi) The AFM ternary diagram to discriminate between calc-alkaline and tholeiitic series ($A = Na_2O + K_2O$, $F = FeO^{\star}$, $M = MgO$). The diagram can be rendered with or without grid, custom symbols and three different symbol sizes. Additionally, the user can select the boundary lines between calc-alkaline and tholeiitic fields proposed by Kuno (1968) or Irvine and Baragar (1971).

vii) The original classification proposed by Shand (1927) based upon Al_2O_3 saturation. The diagram can be rendered with or without grid, custom symbols and three different symbol sizes.



a)



b)

Figure 7: a) An example of the output window after the TAS diagram (Le Maitre et al., 1989) has been produced with medium size symbols (Macintosh version). The dashed line is the subdivision alkaline/sub-alkaline rocks from Irvine and Baragar (1971). b) The Key of the same plot.

viii) The discrimination between calc-alkaline and tholeiitic series in an arc setting based in the ratio FeO/MgO vs. SiO_2 proposed by Miyashiro (1974). The diagram can be rendered with or without grid, custom symbols and three different symbol sizes.

ix) The classification of volcanic rocks proposed by Jensen (1976) according to their cation percentages of Al, $Fe_{total}+Ti$ and Mg, particularly useful for komatiites. PINGU 1.6 renders the modified fields proposed by Rickwood (1989). The diagram can be rendered with or without grid, custom symbols and three different symbol sizes.

x) The classification of "granitic" rocks proposed by Barker (1985), based on molecular normative An, Ab, Or. The diagram can be rendered with or without grid, custom symbols and three different symbol sizes.

xi) The $CaO - MgO - Al_2O_3 - SiO_2$ (CMAS) system developed by O'Hara (1968), projected from olivine in the ternary system diopside-nepheline-quartz. The diagram can be rendered with or without grid, custom symbols and three different symbol sizes.

xii) The normative nepheline-diopside-olivine-quartz tetrahedron introduced by Yoder and Tilley (1962). PINGU first calculates the CIPW norm following Johannsen (1939) and calculates the proportion between the normative minerals before projecting into the tetrahedron. Hypersthene and plagioclase from the norm are allocated in terms of the end-members of the plot (Ne, Ol, Qz, Di) as $ol = ol + 0.7hy$ $ne = ne + 0.5pl$ and $Qz = Qz + 0.3hy + 0.5pl$ (Figure 10). The diagram can be rendered with custom symbols and three different symbol sizes. Alternatively, the projection view can be modified with the Azimuth angle to control the orientation (between 0° and 360° degrees) and the Polar Angle to control the inclination (between 0° and 180° degrees).

xiii) The Rare Earth Element (REE) diagram, normalized using the values reported by Sun and McDonough (1989) C1 chondrite. The diagram can be rendered with or without grid, custom symbols and three different symbol sizes.

xiv) Several styles of spider diagrams introduced originally by Thompson (1982) and Pearce (1983) normalized to MORB, OIB and chondrite values from Sun and McDonough (1989). The diagrams can be rendered with or without grid, custom symbols and three different symbol sizes (Figure 8).

xv) The Nb/Y vs Zr/TiO_2, Nb/Y vs SiO_2 and Zr/TiO_2 vs SiO_2 classification diagrams introduced by Winchester and Floyd (1977). The diagrams can be rendered with or without grid, custom symbols and three different symbol sizes (Figure 9).

xvi) The $Ti - Zr - Y$, $Ti - Zr$ and $Ti - Zr - Sr$ tectonic setting diagrams for tholeiitic basalts introduced by Pearce and Cann (1973). The diagrams can be rendered with or without grid, custom symbols and three different symbol sizes.

xvii) The $Nb - Y$, $Ta - Yb$, $Rb - (Y + Nb)$, $Rb - (Y + Ta)$ tectonic setting diagrams for granites introduced by Pearce et al. (1984). The diagrams can be rendered with or without grid, custom symbols and three different symbol sizes.

Additionally, PINGU can plot any bi-variate and ternary diagram based on the inputted data, selecting the Plot type "Generic X-Y plot" and "Generic Triangular plot" in the Plot Window, respectively. These diagrams can be rendered with or without grid, custom symbols and three different symbol sizes. Bi-variate diagrams can be plotted using a semi-log or a log-log scale, with the x-axis reversed, or with both axes with the same scale for calculations involving the lever rule. If the user intends a more specific diagram (e.g. ratio between variables), these can be done selecting "Custom axis X", "Custom axis Y" and "Custom axis Z" as axes of the generic bi-variate and ternary plots. The data for creating these plots should be located in the last three columns of the input spreadsheet. If custom axes are selected, the user also has the additional capability of adding custom labels to the axes of the given plot.

The Pearce (1983) spider diagram (Figure 8); Winchester and Floyd (1977) Nb/Y vs Zr/TiO_2 diagram (Figure 9); and the Yoder and Tilley (1962) tetrahedron diagram (Figure 10) are shown here as examples of the JPEG output using medium size default symbols.

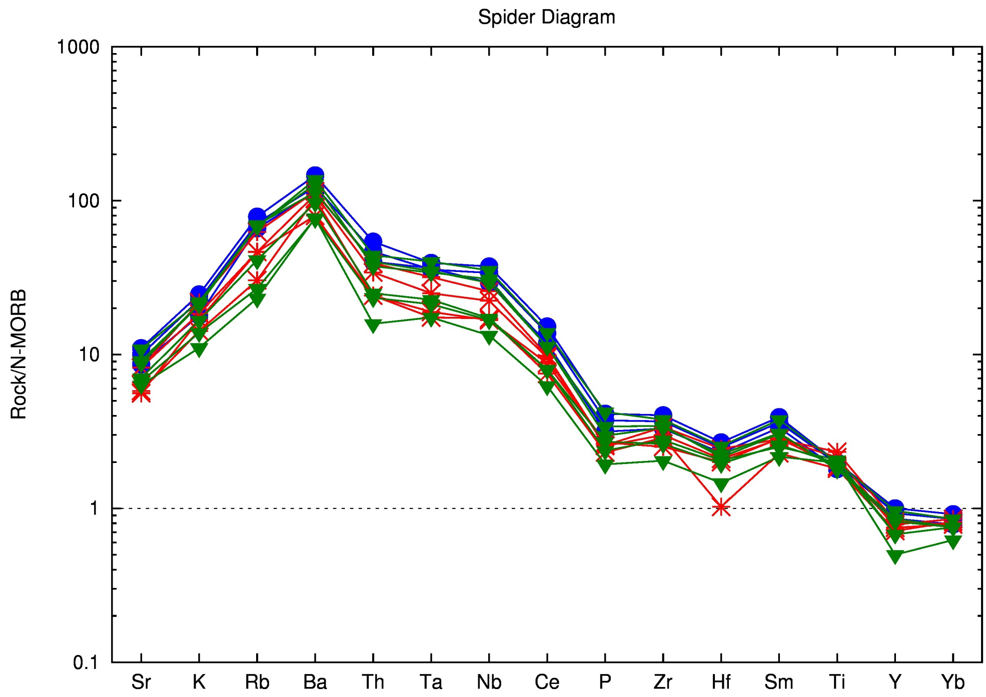


Figure 8: Pearce (1983) spider diagram normalized according to Sun and McDonough (1989)

5. Conclusions

In this contribution we have introduced PINGU 1.6; an online multiplatform tool to produce high-quality EPS or JPEG diagrams, commonly used in igneous petrology and volcanology. The high quality of the plots make the tool suitable for generating diagrams for professional papers, but also for pedagogical purposes in the context of an undergraduate/graduate igneous petrology/volcanology class. PINGU 1.6 only requirements are an Internet connection and an Internet browser with a JAVA plug-in enabled. The tool is constantly updated and expanded by the authors, and actively supported through Vhub resources (the PINGU Appreciation Society) in which manuals and resources can be consulted, and questions, problems and new requests (e.g. the implementation of a new diagram) can be put forward by the users.

Acknowledgements

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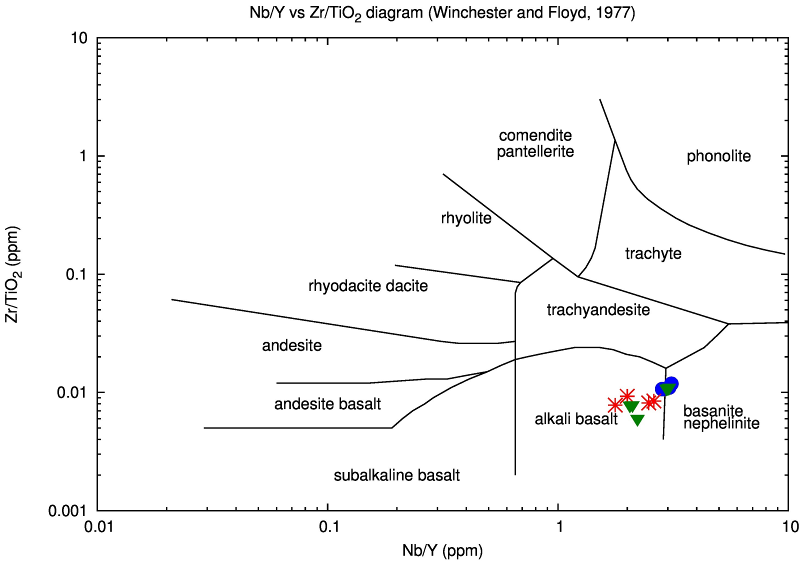

Figure 9: Winchester and Floyd (1977) discrimination diagram

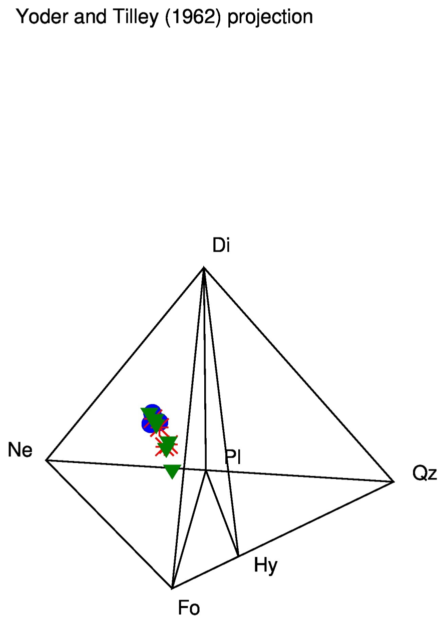

Figure 10: Yoder and Tilley (1962) tetrahedron viewed with an azimuth angle of 309° and polar angle of 67°.

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