# Original paper HafAn: a R-language script aiding interpretation of the Hf isotopic data

# Vojtěch JANOUŠEK\*

Czech Geological Survey, Klárov 3, 118 21 Prague 1, Czech Republic; vojtech.janousek@geology.cz \* Corresponding author



*HafAn* is a new R-language script for recalculation, statistical treatment and graphical presentation of the Hf isotopic data from whole-rock samples or, more commonly, obtained *in situ* (e.g. by LA MC ICP-MS) from igneous, metamorphic and detrital zircon. Besides the recalculation of the present-day Hf isotopic ratios to initial ones, epsilon values and various variants of model ages, it allows presentation of such univariate data in the form of histograms, boxplots, stripplots and violin plots. Arguably the most telling and sophisticated way of displaying the Hf isotopic data are the Hf isotopic growth (age–<sup>176</sup>Hf/<sup>177</sup>Hf or epsilon Hf) diagrams. The *HafAn* has been designed as a plugin module for the *Geochemical Data Toolkit* (aka *GCDkit*), a well-established system for interpretation of the whole-rock geochemical data. This approach potentially allows interpretation (and plotting) of the Hf isotopic data so a single diagram. Moreover, *R/GCDkit* contains a plethora of additional statistical tools that can be newly applied to the Hf isotopic data as well. Our *HafAn* also profits from a wide palette of the file formats available for reading data input, as well as exporting results and graphical output. The *HafAn* plugin, together with all the *GCDkit*-family tools, can be downloaded from *https://gcdkit.org*.

Keywords: Hf isotopes, zircon, software, R language, GCDkit, FOSS Received: 27 February 2024; accepted: 28 June 2024; handling editor: V. Rapprich The online version of this article (doi: 10.3190/jgeosci.391) contains electronic supplementary material.

### 1. Introduction

Since the turn of the millennium, *in-situ* Hf isotope analyses on zircon have become a tool of choice in studies concerned with igneous petrogenesis, sediment provenance or crustal growth (e.g., Belousova et al. 2010; Kemp and Hawkesworth 2014; Cawood et al. 2022). This breakthrough was enabled by the advancement of the Laser-Ablation Multi-Collector Inductively-Coupled Mass Spectrometry (LA MC ICP-MS), routinely producing large and precise Hf datasets. It went hand in hand with progress in *in-situ* U–Pb dating; therefore, Hf isotope data from zircons can be nowadays related to their ages.

However, the interpretation of such datasets requires rather complex recalculations, statistical treatment and specialized plotting (Spencer et al. 2020). Such operations should be performed by a potent and user-friendly computing package. Ideally it should be a Free and Open Source Software (FOSS; Mader and Schenk 2017) written in some common scientific computing language (such as R or Python), enabling subsequent statistical assessment and producing high-quality graphical output.

Indeed, some of such functionality needed for handling the Hf isotopic data from detrital zircons is already builtin in existing programs, most notably the R-language package *detzrcr* (Andersen et al. 2018). In our view, there still remains a scope for a simple, lightweight general package for recalculation of whole-rock and *in-situ* Hf isotopic data that would be easy to use and tweak. For this purpose, it should feature a lucid external configuration file holding recalculation constants that can be effortlessly amended by an ordinary user. Moreover, it should be able to deal with multitude of data formats, and to split the dataset into coherent groups according to various criteria. Lastly it should offer flexible ways of post-processing the recalculated data, including their statistical evaluation and plotting, ideally together with the outstanding geochemical information – be it wholerock or *in-situ* zircon trace-element and/or isotopic data.

For these reasons, we have developed *HafAn*, a package for the interpretation of the Hf isotopic data. It has been designed as a plugin for Geochemical Data Toolkit (aka *GCDkit*), our freeware for te treatment of whole-rock geochemical data from igneous and metamorphic rocks in R (Janoušek et al. 2006, 2016). Using the standard *GCDkit* functionality, the combined Hf and U–Pb data (and the results of their recalculation) can be loaded from (saved in) a multitude of file formats or pasted from (to) the clipboard. The Hf-specific recalculations are accessible from the *Plugin* menu, external R scripts, or can be invoked in direct mode. The results can be post-processed using the powerful statistical and plotting tools (e.g., contour diagrams, spiderplots) available in the *GCDkit* or, more generally, the R with its contributed packages.

### 2. Interpretation of Hf isotopic data

The Lu–Hf method relies on  $-\beta$  decay of <sup>176</sup>Lu to <sup>176</sup>Hf (Boudin and Deutsch 1970) with a half-life of *c*.  $3.72 \times 10^{10}$  yr (Scherer et al. 2001; Hayakawa et al. 2023). In practise, abundances of these isotopes are expressed relative to the stable <sup>177</sup>Hf, leading to the following equation:

$$\left(\frac{^{176}Hf}{^{177}Hf}\right)_{0} = \left(\frac{^{176}Hf}{^{177}Hf}\right)_{t} + \frac{^{176}Lu}{^{177}Hf}\left(e^{\lambda t} - 1\right)$$
(1)

where  $\lambda$  is the decay constant,  $\theta$  refers to the present, t to the time when the "radioactive clock" has started (e.g. magma crystallization) and  $({}^{176}\text{Hf}/{}^{177}\text{Hf})_t$  is known as the initial ratio.

Similarly to the Sm–Nd system (DePaolo 1988), the so-called Chondritic Uniform Reservoir (CHUR) is widely used for comparison of initial Hf isotopic compositions of the studied sample (SA) with that of chondritic (= primitive, i.e. undifferentiated) mantle at the time of their generation (Patchett et al. 1982; Blichert-Toft and Albarède 1997). For this purpose serves the  $\varepsilon_{\rm Hf}$  notation:

$$\varepsilon_{Hf}^{t} = \left(\frac{\left(\frac{176}{177}Hf\right)_{t}^{8.4}}{\left(\frac{176}{177}Hf\right)_{t}^{CHUR}} - 1\right) \times 10^{4}$$
(2)

This leads to a concept of model ages, that simply represent an apparent extraction age from some canonical mantle reservoir, most typically CHUR or Depleted Mantle (DM) (Fig. 1a). In the former case, a singlestage Hf model age is calculated as follows (Faure and Mensing 2004):

$$T_{Hf^{1}stg}^{DM} = \frac{1}{\lambda} \ln \left[ \frac{\left( \frac{176}{177} Hf}{177} \right)_{SA}^{0} - \left( \frac{176}{177} Hf}{0} \right)_{CHUR}^{0} + 1 \right]$$
(3)

If interpreting sources of crustally-derived rocks (e.g., granitoids), the single-stage model ages are inappropriate. Since we do not know the <sup>176</sup>Lu/<sup>177</sup>Hf ratio of the source from which magma parental to the studied



**Fig. 1a** – Theoretical concept of a single-stage Hf model age as an intersection between the evolution lines of the mantle (here the CHUR) and that for the given sample. **b** – Principle of the two-stage Hf model age. An intermediate reservoir with Lu/Hf ratio of selected typical continental crustal reservoir (*CC*) is to be assumed. For explanation, see the text.

zircon was generated, some reasonable assumption has to be made. In principle this ratio can vary rather widely, between the postulated average felsic upper continental crustal ( $\sim 0.010$ ) and mafic lower crustal values ( $\sim 0.026$ ) (Spencer et al. 2020) (Fig. 1b). The two-stage model age calculations essentially employ the approach of Liew and Hofmann (1988), adopted for the zircon Hf analysis (Andersen et al. 2002; Kemp and Hawkesworth 2003).

$$T_{H_{2}2xg}^{DM} = \frac{1}{\lambda} \ln \left[ \frac{\left(\frac{176}{H_{f}}H_{f}}{177}\right)_{S4}^{0} - \left(e^{\lambda t} - 1\right) \left[ \left(\frac{176}{Lu}\right)_{S4}^{0} - \left(\frac{176}{177}H_{f}}\right)_{CC}^{0} - \left(\frac{176}{177}H_{f}}\right)_{DM}^{0} + 1 \right] \left(\frac{176}{177}H_{f}}{\left(\frac{176}{177}H_{f}}\right)_{CC}^{0} - \left(\frac{176}{177}H_{f}}\right)_{DM}^{0} + 1 \right]$$

where CC refers to the putative crustal source and t to the zircon crystallization age.

### 3. Program description

### 3.1. Data format

The combined Hf and U-Pb data can be loaded from the *GCDkit* menu, invoking items *Load data file* (attached to the function loadData()) or *Paste data from clipboard*. The supported file formats include plain-text (\*.TXT, \*.CSV), MS Excel (\*XLS(X)), MS Access (\*.MDB) and dBase (\*.DBF). Sample datasets can be loaded from the menu *GCDkit*|*Sample dataset* (attached to the function sampleDataset()).

The files are close to freeform with individual analyses in rows and variables in columns. Still, they should always contain at least the columns '176Lu/177Hf' and '176Hf/177Hf'. Optional is a column 'Age' (in Ma), as are any textual columns - such as those specifying the sample number or locality - that can be used for grouping and/or assigning plotting symbols or colours. Moreover, plotting attributes can be pre-defined in the datafile, in columns 'Symbol', 'Colour' and/ or 'Size'.

Note that the datafile is essentially a database, so both the row names (taken from the first column of the file) and column names (taken from the first row) need to be unique. This requirement can be bypassed, e.g., by using sequence numbers as the first column in the datafile. Alternatively, Excel (\*.XLS/\*.XLSX) import filter is clever enough to import such files, assigning the sequence numbers automatically. See the sample datasets and current documentation to the GCDkit package for further information.

**Fig. 2a** – Menu of the *HafAn* plugin. **b** – Screenshot of the graphical (Tcl/Tk) editor for constants used for calculations.

### 3.2. Data recalculation procedure

Upon loading a new dataset, the data are automatically recalculated to initial  $^{176}\mathrm{Hf}/^{177}\mathrm{Hf}$  ratios (function

See/change calculat	tion parameters
Recalculate to new	age
Copy Hf isotopic da	ata to clipboard
Save Hf isotopic dat	ta
Append Hf isotopic	data
Hafnium DM growt	h lines
Histogram ages/iso	topic ratios/model ages
Boxplot ages/isotop	pic ratios/model ages
Stripplot ages/isoto	pic ratios/model ages
/iolinplot ages/isot	opic ratios/model ages
N: 1 1 1	
lichlay ledend	



(a)

hfInitial()), initial  $\varepsilon_{\rm Hf}$  values (hfEpsilon()), single-stage CHUR (hfCHURage()) and depletedmantle (hfDMage()) model ages, as well as two-stage DM model ages (hfDM2stgAge()). All of these computations are invoked by the wrapper function hfIso(). Moreover, when the Hf isotopic data are recognized and recalculated, a new item *'Hf isotopes'* appears in the menu *Plugin* (Fig. 2a). If ages of individual zircons are defined in the data file, these will be used for calculation of Hf initial isotopic compositions. If the parameter 'age' is provided upon the call to the *HafAn* master function hflso(), an identical value is employed for all the samples. On the other hand, if the parameter 'age' is not set, and no column named 'Age' is present in the dataset, the user is prompted to enter a common value via a dialogue box.



Fig. 3 Statistical plots for U-Pb ages and Hf isotopic parameters available in *HafAn*. Data from the Cambrian Khantaishir Magmatic Complex (Lake Zone, Mongolia) (Janoušek et al. 2018) (file 'khantaishir\_Hf') have been used as an example. **a** – Frequency histogram of U-Pb ages, **b** – Boxplot of two-stage DM model ages, **c** – Stripplot of the same, **d** – Violin plot of single-stage DM model ages.

### 3.3. Grouping

An important concept for data treatment in *GCDkit* is grouping, defining groups of analyses that belong together based on some criterion. As outlined in the *GCDkit* documentation, the desired mechanism can be chosen from the menu *Data handling*|*Set groups by*.... Arguably most convenient is grouping based on some textual column in the datafile (aka a label: e.g., sample name, intrusion/ geological unit or region) linked to the option ... *by label*.

### 3.4. Graphics

#### 3.4.1. Univariate statistical plots

Statistical plots are employed to elucidate the statistical distribution of U–Pb ages or of a single Hf isotopic parameter, for the whole dataset or separately, by groups. The Hf isotopic parameters that can be plotted include the U–Pb ages, initial <sup>176</sup>Hf/<sup>177</sup>Hf and  $\varepsilon_{\rm Hf}$  values, and various variants of the model ages.

*Histograms* The frequency histogram implemented in *HafAn* is merely a front-end to the standard R function *hist()*. In addition, a curve denoting the kernel density estimate (calculated by the R function *density()*) can be overplotted (Fig. 3a).

*Boxplots* The boxplot (or box-and-whisker plot) has been designed by Tukey (1977) to portray a statistical distribution of univariate data. The box represents, for each of the groups, the two quartiles, the line inside is a median, and the whiskers show the whole range without outliers (Fig. 3b). The outliers themselves are shown by small circles.

*Stripplots* Stripplot (Esty and Banfield 2003) shows 1D scatter plots for each of the groups, with some artificial noise (jitter) added to make the individual points better visible (Fig. 3c). Stripplots are a good alternative to boxplots when sample sizes are small, so are ideal for isotope geology.

*Violin plots* Violin plots have been proposed as yet another alternative to boxplots for illustrating the distribution of univariate statistical data (Hintze and Nelson 1998). In effect they combine boxplot with two density traces placed symmetrically around it (Fig. 3d). The box extends between the two quartiles; median is denoted by a point. The whiskers show the whole range without outliers. However, unlike in the boxplots, outliers are not shown as individual points.

# 3.4.2. Hafnium evolution diagrams (t(U–Pb) vs. $\epsilon_{_{Hf}}$ plots)

Single- or two-stage Hf growth curves in individual samples can be shown on the t(U–Pb) vs.  $^{176}$ Hf/ $^{177}$ Hf or  $\epsilon_{\rm Hf}$  plots (Kemp and Hawkesworth 2003, 2014). The x

axis, t(U–Pb), is either the  ${}^{206}Pb/{}^{207}Pb$  or  ${}^{206}Pb/{}^{238}U$  age of the individual zircon grains (Fig. 4). Alternatively, it can be a 'preferred age'; e.g.  ${}^{206}Pb/{}^{238}U$  age for the zircons younger than 1 Ga and  ${}^{206}Pb/{}^{207}Pb$  age for the older ones.

Superimposed are Hf growth curves for the two main model mantle reservoirs, CHUR and Depleted Mantle (DM) that can be either a single- or two-stage (Fig. 4a–b). Optionally, the small ticks, or rug, on the x axis may correspond to Hf model ages (single- or two-stage, respectively); rug on the y axis portrays the initial <sup>176</sup>Hf/<sup>177</sup>Hf or  $\varepsilon_{\rm Hf}$  values (Fig. 4a–e). Optionally, violin plots can be added portraying statistical distribution within each group (Fig. 4c). Moreover, frequency histogram of U–Pb ages may be displayed at the bottom of the Hf growth diagram, with kernel density curve calculated by the R function *density()* (Fig. 4d–f) and assuming KDE bandwidth ( $\sigma$ ) of 30 as a default (Vermeesch and Garzanti 2015; Andersen et al. 2018).

Note that the Hf isotope growth diagrams are Figarocompatible (Janoušek et al. 2006). This means that each of these diagrams is stored as an object in memory and thus can be post-processed from the standard *GCDkit* menu *Plot editing*. For instance one can change the graph limits, scale plotting symbols/axis labels, or change the plotting symbols/colours. Lastly, contours (Fig. 4e) or filled contours (Fig. 4f) can be added, in the former case for the entire dataset or respecting the grouping.

#### 3.5. Exporting data and graphics

The results of calculations can be saved into a text file using the function hfSaveResults(). Supported are also WWW pages (\*.HTML) and Microsoft Excel (\*XLS) files; results can be also pasted to the clipboard. The graphics may be exported into a number of vector-(PostScript, PDF and WMF) and bitmap-based (e.g., PNG, TIF and JPG) formats, which can be imported into a professional graphical editor for further editing.

### 3.6. Setting up constants for recalculations

The constants used for Hf isotopic data recalculations are chosen via the graphical user interface (GUI) (Fig. 2b), which is triggered by the function hfOptions(). These include the <sup>176</sup>Lu decay constant (Tatsumoto et al. 1981; Sguigna et al. 1982; Scherer et al. 2001; Söderlund et al. 2004; Hayakawa et al. 2023), the <sup>176</sup>Lu/<sup>177</sup>Hf and <sup>176</sup>Hf/<sup>177</sup>Hf ratios of the canonical CHUR (Blichert-Toft and Albarède 1997; Bouvier et al. 2008) and DM (Griffin et al. 2002; Vervoort et al. 2018) reservoirs, as well as the crustal <sup>176</sup>Lu /<sup>177</sup>Hf ratio to be employed in the calculation of the two-stage Hf model ages. The latter may represent the average bulk continental crust (Rudnick and Gao 2003), upper continental crust (Chauvel et al. 2014;



Spencer et al. 2020), lower continental crust (Spencer et al. 2020) or basaltic crust (Lancaster et al. 2011). For time being, our GUI editor allows only choosing, but not adding/editing the parameters. With reasonable care, such changes can be made directly in the plain-text configuration file 'constants\_hflso.xxx' with a simple structure. Just note that the default/currently selected options are preceded by an asterisk.

### 3.7. Sample dataset – Khantaishir Magmatic Complex (Lake Zone, Mongolia)

As the first sample dataset distributed with the *HafAn* plugin serves the file 'khantaishir\_Hf.csv', which translates to a data frame containing 111 zircon analyses (Lu-Hf isotopes and U-Pb ages) of 5 samples of mafic-intermediate plutonic rocks from the Cambrian Khantaishir Magmatic Complex (Lake Zone, Mongolia) (Janoušek et al. 2018). It represents a section of a magmatic arc system consisting of deep crustal, (ultra-)mafic cumulates (coarse-grained amphibole gabbros and hornblendites) to shallower crustal levels dominated by amphibole-biotite tonalites. These Hf-in-zircon isotopic data, together with whole-rock Sr-Nd isotopic compositions, point mostly to juvenile sources, with little, if any, mature crustal contribution.

The second sample file contains 179 Lu–Hf isotopic analyses and U–Pb ages of detrital zircons from five metasedimentary samples of the Tatric Unit (Western Carpathians, Slovakia: Soejono et al. 2018).

# 4. A sample session: using *HafAn* in direct (or batch) mode

Apart from the menus, *HafAn* functions can be also invoked directly, either interactively (from command prompt) or in batch mode (allowing scripting for automated use). The latter approach is useful for productivity (working with mutating or multiple datasets) as well as reproducibility (documenting the recalculation procedure applied to the given dataset); it also allows fine tuning the arguments to individual functions. In the following

 $\Diamond$ 

text, we shall demonstrate the power (and sheer beauty) of this approach.

To start with, we load the Khantaishir sample dataset, using a dedicated function:

```
sampleDataset("khantaishir_Hf")
head(WR)
head(labels)
```

Note that ordinary datasets would need to be loaded by the function loadData.

Upon loading a new dataset, the data are recalculated automatically to the ages specified in the input file, and the result is stored in a dataframe Hfinit:

head(Hfinit)

From now on, the functions for calculation of the initial Hf isotopic ratios, epsilon Hf values and model ages can be invoked directly, with new recalculation parameters as arguments. Such computations do not affect the Hfinit object, though:

```
hfInitial(346)
head(cbind(hfEpsilon(0),
    hfEpsilon (500)))
head(cbind(hfCHURage(),hfDMage()))
hfDM2stgAge(age = 300)
hfDM2stgAge(RCC = 0.022)
    # Basaltic RCC
    # (Lancaster et al. 2011)
```

Grouping the analyses according to the sample they belong to:

```
groupsByLabel("sample")
```

we can have a look on statistical distribution of U–Pb ages and selected Hf isotopic parameters in each of them:

```
hfHist("Age (Ma)", bin.width = 10,
    col = "khaki", kde = TRUE,
    kde.bandwidth = 30)
hfBoxplot("HfTDM.2stg", cex.axis= 1,
    col = heat.colors(5))
hfStripplot("HfTDM.1stg")
hfViolinplot("EpsHfi",
    col = "lightblue")
```

Arguably the best way of presenting Hf isotopic data are the t(U–Pb) vs.  $^{176}\rm Hf/^{177}\rm Hf$  or  $\epsilon_{\rm Hf}$  plots. Here are examples of two-stage Hf growth curves:

```
hfAgeEps1(1:39, xmin = 0.4,
    xmax = 0.6, rugs = FALSE,
    evol.lines1 = TRUE,
    evol.lines2 = FALSE)
hfAgeHfHf2(1:39, xmax = 1.5,
    evol.lines1 = TRUE,
    evol.lines2 = FALSE)
hfAgeEps2(1:39, xmin = 0.4,
    xmax = 0.6, rugs = FALSE,
    age.hist = TRUE,
    kde.bandwidth = 30)
hfLegend("topleft")
```

**Fig. 4** Examples of the Hf evolution plots, i.e. binary plots of U–Pb age vs.  $\varepsilon_{\rm Hf}$  or <sup>176</sup>Hf<sup>/177</sup>Hf. **a** – Single-stage growth model, **b**–**f** Two-stage growth models. Extra ticks (rugs) on x and y axes depict the model ages and initial  $\varepsilon_{\rm Hf}$  values or initial <sup>176</sup>Hf<sup>/177</sup>Hf for individual analyses. In (d–f), frequency histogram of the U–Pb ages (Ma) is also shown (a KDE curve assuming kde.bandwidth = 30). In (e), contours have been added (levels = c(0.05, 0.01) respectively leaving out 5% and 1% of the dataset behind the contour), while (f) demonstrates the filled contour plot. Data in a–c are from the Cambrian Khantaishir Magmatic Complex (Lake Zone, Mongolia; Janoušek et al. 2018), in d–f from detrital zircons of metavolcanic–sedimentary basement in the Western Carpathians (Slovakia; Soejono et al. 2024).

and such a diagram can be contoured by the standard *GCDkit* tools:

```
hfAgeEps2(xmax = 1.5, ymin = -8,
    ymax = 16, evol.lines2 = FALSE)
figXlim(c(0.4,0.7))
figYlim(c(0,16))
addContours(col = "darkgray",
    lty = "dashed")
```

It is worth noting that the function addContours accepts all the arguments of the R function contour, see help (?contour). For instance, parameter levels gives percentages of samples falling outside of the given contour line. Logical parameter drawlabels determines whether they are to be labelled, or not.

Moreover, each of the groups can be contoured separately:

```
figRedraw()
contourGroups()
Filled contours can be obtained as follows:
filledContourFig(palette =
    "heat.colors", grid.density =
    20, overplot = TRUE)
```

# 5. Summary and outlook

The brand new plugin *HafAn* represents a simple, yet versatile and customizable addition to the *GCDkit* R package. Over the years, the *GCDkit* became established standard in interpretation of geochemical data from igneous and metamorphic rocks (Janoušek et al. 2023). Thanks to the *HafAn*, tools for interpretation of the U–Pb ages and/or Hf isotopic data are now available from a familiar graphical user interface and thus should be easy to learn and utilise.

The *HafAn* plugin represents a simple, lightweight software. Only for production of violin plots it relies on the *vioplot* R package by Adler et al. (2022), with its two dependencies, *sm* and *zoo*. This is in contrast to specialised and inherently complex R packages designed specifically for provenance analysis, using the age spectra and/ or Hf isotopic chemistries of detrital zircons. While the *provenance* package (Vermeesch et al. 2016; Vermeesch 2024) excels in plotting and statistical treatment of detrital U–Pb ages, *detzrcr* (Andersen et al. 2018; Kristoffersen 2022) is capable of dealing with both univariate (U–Pb ages) and bivariate (U–Pb ages and Hf isotopic compositions) zircon data.

Notable is the seamless integration of *HafAn* into the *GCDkit* system. The function hfAddResults() linked to the menu *Append Hf isotopic data* adds the calculated

Hf isotopic parameters (data frame Hfinit) to the variable WR of the GCDkit. For whole-rock datasets, this allows a combination of Hf isotopic compositions with the major- and trace-element data, and/or other isotopic ratios (e.g. <sup>143</sup>Nd/<sup>144</sup>Nd). For the *in-situ* zircon data, it opens the possibility of including any possible extra compositional information (whenever available) into interpretation, be it, for instance, trace-element and/or O isotope data. Such combined datasets can then be visualised and evaluated using rich graphical and statistical tools available in the GCDkit: for example, multivariate statistics, spiderplots or contour plots (Janoušek et al. 2016). There is also a tempting possibility of merging or overplotting multiple Hf isotopic datasets onto a single diagram, facilitating comparisons. For these reasons, we believe that the HafAn plugin will be able to find its interested users.

# 6. Availability and installation

The first version of the *HafAn* plugin and accompanying documentation can be downloaded from the Journal web page, *http://dx.doi.org/10.3190/jgeosci.391*. Note that *HafAn* is a plugin to the R package *GCDkit*, whose version 6.2.0 (or above) needs to be correctly installed. The current releases for the entire *GCDkit* family of tools can be downloaded from *https://gcdkit.org*.

To install *HafAn*:

- Unpack the 'HafAn\_install.zip' archive (ESM 1) into a convenient temporary directory.
- Run RGUI, 32 bit version (shortcut labelled *R i386* on your desktop).
- Drag and drop the file <code>@Hf\_OFFLINE\_INSTALL.r</code> from the temporary installation directory onto the R Console window. Otherwise, the <code>@Hf\_OFFLINE\_INSTALL.r</code> file can be also located and run using *File>Source R code...* menu of R.
- Wait till the installation completes, the process should be fully automatic:
  - The support library/ies (including their dependencies) are installed from the temporary directory (no Internet connection is required).
  - GCDkit 6.2.0 is patched, if necessary.
  - The *HafAn* Plugin is installed, and the help system of *GCDkit* updated.
- (Restart R/GCDkit).

In the future releases of the *GCDkit* system (i.e., starting with the version 6.3.0.), *HafAn* will be embedded as a standard plugin and, therefore, no separate installation will be required anymore.

Running is also easy. The *HafAn* plugin is loaded automatically, as soon as a file with Hf isotopic data is encountered. The documentation to individual func-

tions is incorporated into the *GCDkit* help system. For the convenience sake, the reference manual is provided in ESM 2. To an interested reader, the Khantaishir and West Carpathian datasets (accessible from the menu *GCDkit*|*Sample dataset*) can serve to test drive our new software.

Acknowledgements. Development of the HafAn plugin has been supported by the Grant Agency of the Czech Republic (GACR) project 22-34175S. This is a contribution to the Strategic Research Plan of the Czech Geological Survey (DKRVO/ČGS 2023–2027) through internal project No. 311330. We are indebted to I. Soejono and R. Anczkiewicz for kind and thought-provoking reviews that helped to improve both the software and this text. Lastly, the author would like to thank Editor-in-Chief V. Rapprich for editorial handling.

*Electronic supplementary material.* The *HafAn* plugin and accompanying manual are available online at the Journal web site (*http://dx.doi.org/10.3190/jgeosci.391*).

## References

- ANDERSEN T, GRIFFIN WL, PEARSON NJ (2002) Crustal evolution in the SW part of the Baltic Shield: the Hf isotope evidence. J Petrol 43: 1725–1747
- ANDERSEN T, KRISTOFFERSEN M, ELBURG MA (2018) Visualizing, interpreting and comparing detrital zircon age and Hf isotope data in basin analysis – a graphical approach. Basin Res 30: 132–147
- BELOUSOVA EA, KOSTITSYN YA, GRIFFIN WL, BEGG GC, O'REILLY SY, PEARSON NJ (2010) The growth of the continental crust: constraints from zircon Hf-isotope data. Lithos 119: 457–466
- BLICHERT-TOFT J, ALBARÈDE F (1997) The Lu-Hf isotope geochemistry of chondrites and the evolution of the mantle-crust system. Earth Planet Sci Lett 148: 243-258
- BOUDIN A, DEUTSCH S (1970) Geochronology: recent development in the lutetium-176/hafnium-176 dating method. Science 168: 1219–1220
- BOUVIER A, VERVOORT JD, PATCHETT PJ (2008) The Lu–Hf and Sm–Nd isotopic composition of CHUR: constraints from unequilibrated chondrites and implications for the bulk composition of terrestrial planets. Earth Planet Sci Lett 273: 48–57
- CAWOOD PA, CHOWDHURY P, MULDER JA, HAWKESWORTH CJ, CAPITANIO FA, GUNAWARDANA PM, NEBEL O (2022) Secular evolution of continents and the Earth system. Rev Geophys 60: e2022RG000789
- CHAUVEL C, GARÇON M, BUREAU S, BESNAULT A, JAHN BM, DING ZL (2014) Constraints from loess on the Hf–Nd

isotopic composition of the upper continental crust. Earth Planet Sci Lett 388: 48–58

- DEPAOLO DJ (1988) Neodymium Isotope Geochemistry. Springer, Berlin, pp 1–187
- ESTY WW, BANFIELD JD (2003) The box-percentile plot. J Stat Softw 8: 1–14
- FAURE G, MENSING TM (2004) Isotopes: Principles and Applications. Wiley, New Jersey, pp 1–928
- GRIFFIN WL, WANG X, JACKSON SE, PEARSON NJ, O'REILLY SY, XU X, ZHOU X (2002) Zircon chemistry and magma mixing, SE China: in-situ analysis of Hf isotopes, Tonglu and Pingtan igneous complexes. Lithos 61: 237–269
- HAYAKAWA T, SHIZUMA T, IIZUKA T (2023) Half-life of the nuclear cosmochronometer <sup>176</sup>Lu measured with a windowless 4p solid angle scintillation detector. Commun Phys 6: 299
- HINTZE JL, NELSON RD (1998) Violin plots: a box plot–density trace synergism. Am Stat 52: 181–184
- JANOUŠEK V, FARROW CM, ERBAN V (2006) Interpretation of whole-rock geochemical data in igneous geochemistry: introducing Geochemical Data Toolkit (GCDkit). J Petrol 47: 1255–1259
- JANOUŠEK V, MOYEN JF, MARTIN H, ERBAN V, FARROW CM (2016) Geochemical Modelling of Igneous Processes – Principles and Recipes in R Language. Bringing the Power of R to a Geochemical Community. Springer, Berlin, pp 1–346
- JANOUŠEK V, JIANG YD, BURIÁNEK D, SCHULMANN K, HANŽL P, SOEJONO I, KRÖNER A, ALTANBAATAR B, ERBAN V, LEXA O, GANCHULUUN T, KOŠLER J (2018) Cambrian–Ordovician magmatism of the Ikh-Mongol Arc System exemplified by the Khantaishir Magmatic Complex (Lake Zone, south-central Mongolia). Gondwana Res 54: 122–149
- JANOUŠEK V, MOYEN JF, MAYNE MJ, FARROW CM, ERBAN V (2023) The R language: an ultimate recalculation, plotting and modelling environment in igneous geochemistry (GCDkit turns twenty!). In: DOUCELANCE R, GARGAUD M, GUITREAU M, MOYEN JF, ROSE-KOGA E, SAMANIEGO P (eds) Granitoids, Continents, Life and Puns. A Tribute to Hervé Martin. Clermont-Fd, 5–8<sup>th</sup> July 2023. Université Clermont Auvergne, Clermont-Ferrand, pp 17
- KEMP AIS, HAWKESWORTH CJ (2003) Granitic perspectives on the generation and secular evolution of the continental crust. In: HOLLAND HD, TUREKIAN KK (eds) Treatise on Geochemistry vol. 3, The Crust (ed. RL RUDNICK). Elsevier-Pergamon, Oxford, pp 349–410
- KEMP AIS, HAWKESWORTH CJ (2014) Growth and differentiation of the continental crust from isotope studies of accessory minerals. In: HOLLAND HD, TUREKIAN KK (eds) Treatise on Geochemistry (Second Edition). Elsevier, Oxford, pp 379–421
- LANCASTER PJ, STOREY CD, HAWKESWORTH CJ, DHUIME B (2011) Understanding the roles of crustal growth and preservation in the detrital zircon record. Earth Planet Sci Lett 305: 405–412

LIEW TC, HOFMANN AW (1988) Precambrian crustal components, plutonic associations, plate environment of the Hercynian Fold Belt of Central Europe: indications from a Nd and Sr isotopic study. Contrib Mineral Petrol 98: 129–138

MADER D, SCHENK B (2017) Using Free/Libre and Open Source software in the geological sciences. Austr J Earth Sci 110: 142–161

PATCHETT PJ, KOUVO O, HEDGE CE, TATSUMOTO M (1982) Evolution of continental crust and mantle heterogeneity: evidence from Hf isotopes. Contrib Mineral Petrol 78: 279–297

- RUDNICK RL, GAO S (2003) The composition of the continental crust. In: HOLLAND HD, TUREKIAN KK (eds) Treatise on Geochemistry vol. 3, The Crust (ed. RUDNICK RL). Elsevier-Pergamon, Oxford, pp 1–64
- SCHERER E, MÜNKER C, MEZGER K (2001) Calibration of the lutetium-hafnium clock. Science 293: 683–687
- SGUIGNA AP, LARABEE AJ, WADDINGTON JC (1982) The half-life of  $^{176}$ Lu by a  $\lambda$ - $\lambda$  coincidence measurement. Can J Phys 60: 361–364
- SöDERLUND U, PATCHETT PJ, VERVOORT JD, ISACHSEN CE (2004) The <sup>176</sup>Lu decay constant determined by Lu–Hf and U–Pb isotope systematics of Precambrian mafic intrusions. Earth Planet Sci Lett 219: 311–324
- SOEJONO I, COLLETT S, KOHÚT M, JANOUŠEK V, SCHULMANN K, BUKOVSKÁ Z, NOVOTNÁ N, ZELINKOVÁ T, MÍKOVÁ J, HORA JM, VESELOVSKÝ F (2024) Paleogeography of the Gondwana passive margin fragments involved in the Variscan and Alpine collisions: perspectives from metavolcanic–sedimentary basement of the Western Carpathians. Earth Sci Rev 253: 104763
- SPENCER CJ, KIRKLAND CL, ROBERTS NMW, EVANS NJ, LIEBMANN J (2020) Strategies towards robust interpreta-

tions of in situ zircon Lu-Hf isotope analyses. Geosci Front 11: 843-853

- TATSUMOTO M, UNRUH DM, PATCHETT PJ (1981) U–Pb and Lu–Hf systematics of Antarctic meteorites. Mem Natl Inst Polar Res (Japan), spec issue 20: 237–249
- TUKEY JW (1977) Exploratory Data Analysis. Pearson, Reading, MA, pp 1–712

VERMEESCH P, GARZANTI E (2015) Making geological sense of 'Big Data' in sedimentary provenance analysis. Chem Geol 409: 20–27

VERMEESCH P, RESENTINI A, GARZANTI E (2016) An R package for statistical provenance analysis. Sediment Geol 336: 14–25

VERVOORT JD, KEMP AIS, FISHER CM (2018) Hf isotope constraints on evolution of the depleted mantle and growth of continental crust. AGU Fall Meeting Abstract #V23A-07

### Web links

- ADLER D, KELLY ST, ELLIOTT T, ADAMSON J (2022) vioplot: violin plot. R package version 0.4.0. Accessed on February 16, 2024, at *https://github.com/TomKellyGenetics/* vioplot
- JANOUŠEK V (2024) GeoChemical Data toolkit (GCDkit) version 6.2. Accessed on June 14, 2024, at https://gcdkit.org
- KRISTOFFERSEN M (2022) detzrcr. R package version 0.3.1. Accessed on February 16, 2024, at *https://github.com/ magnuskristoffersen/detzrcr*
- VERMEESCH P (2024) provenance: an R package for statistical provenance analysis. Accessed on May 14, 2024, at https://www.ucl.ac.uk/~ucfbpve/provenance