

UThwigl - an R package for closed- and open-system uranium-thorium dating

Anthony Dosseto^a, Ben Marwick^b

^a*Wollongong Isotope Geochronology Laboratory, School of Earth, Atmosphere & Life Sciences, University of Wollongong, Wollongong NSW Australia*

^b*Department of Anthropology, University of Washington, Seattle, WA, USA*

Abstract

For several decades, uranium-thorium (U-Th) dating has allowed geochronologists to precisely date geological materials, providing invaluable geochronological constraints on Quaternary processes. Open-system dating of bones and teeth has also provided ages of human and faunal remains of archaeological significance.

To facilitate access of open-system U-Th dating to the broad scientific community, here we provide an R package, named *UThwigl*, that implements the Diffusion-Adsorption-Decay model of Sambridge et al. (2012). Description of input and output parameters is given, as well as a guide for running the model. The package can be used three different ways: (i) as a web application, (ii) through a web browser with an internet connection, or (iii) in R (most efficiently with RStudio). Examples of application of the model are also provided, showing that it yields ages within error of previously published values.

Email addresses: tonyd@uow.edu.au (Anthony Dosseto), bmarwick@uw.edu (Ben Marwick)

1 Introduction

2 Uranium-thorium (U-Th) dating has revolutionised Quaternary science and
3 archaeology. Dating uses the decay of ^{238}U into ^{230}Th , with ^{234}U and a few
4 short-lived nuclides as intermediary products. It is based on the principle that
5 the age of formation of a material can be dated as it incorporates U and no or
6 little Th at the time of formation, so all the ^{230}Th in the sample comes from
7 decay of ^{238}U . If detrital Th is included to the sample, a correction must be
8 included to account for the fraction of ^{230}Th which is detrital and not derived
9 from ^{238}U decay. Another requirement is that there is no gain or loss of ^{230}Th ,
10 ^{234}U or ^{238}U after formation of the material (*closed system*).

11 Closed-system U-Th dating has been successfully applied to a range of
12 carbonates, from corals (Edwards, Gallup, and Cheng 2003) to speleothems
13 (Richards and Dorale 2003). In corals and most speleothems, detrital correction
14 is minimal; however, it can be significant when dating pedogenic carbonates,
15 for instance (Ludwig and Paces 2002). In this case, detrital correction can
16 be performed using the measured or assumed composition of the detrital frac-
17 tion (e.g. K. Ludwig 2003). Alternatively, isochron techniques can be applied
18 (Ludwig and Titterton 1994); the latter are beyond the scope of this article
19 but IsoPlot is a commonly used software for isochron calculations and other
20 geochronological applications (K. R. Ludwig 2003).

21 Closed-system conditions are seldom met in teeth and bones (although enamel
22 can sometimes be quite impervious to isotope gain or loss). Thus, for teeth and
23 bone, U-Th dating requires to take into account open system behaviour. The
24 diffusion-adsorption-decay (DAD) model developed by Sambridge et al. (2012)
25 was instrumental to implement successfully open-system U-Th dating. It allows
26 for advective and diffusive transport of uranium and thorium isotopes, while
27 include synchronous radioactive decay. The software implementation was writ-
28 ten in Fortran and is available as a Java GUI ([http://www.earth.org.au/codes/](http://www.earth.org.au/codes/iDaD/)
29 [iDaD/](http://www.earth.org.au/codes/iDaD/)).

30 Open-system U-Th dating of teeth and bones, while challenging, has pro-
31 vided quantitative ages for human and faunal remains (Eggins et al. 2005;
32 Grün et al. 2014; Sambridge, Grün, and Eggins 2012). Thus, this approach has
33 significantly improved our understanding of human evolution (e.g. Dirks et al.
34 2017; Sutikna et al. 2016).

35 In this article, we propose a R package which offers functions to perform
36 closed-system, `csUTh()`, and open-system, `osUTh()`, U-Th age calculations. The
37 former implements formulations given in Ludwig (2003) while the latter applies
38 the Diffusion-Adsorption-Decay (DAD) model of Sambridge et al. (2012). The
39 motivation for providing an R package is to increase the transparency, repro-
40 ducibility, and flexibility of the analytical workflow for computing U-Th ages.
41 For instance, with open-system dating, it is difficult to include the Java GUI in a
42 fully scripted data analysis so the method for computing the DAD model is not
43 highly transparent. This can obscure steps where key decisions are made that
44 are important for others to see to verify the reliability of the analysis. Enabling
45 a scripted workflow for computational analysis of geoscience data is important

for improving the reproducibility of results. Reproducibility refers the ability to recreate the results or retest the hypotheses leading to a scientific claim, either by rerunning the same code used by the original authors, or by writing new code. High rates of irreproducibility of research results have been estimated in several fields and disciplines (Medical Sciences 2015; Freedman, Cockburn, and Simcoe 2015; Institute 2013; Ioannidis 2005; Collaboration and others 2015; Camerer et al. 2018, 2016). Consequently, the transparency, openness, and reproducibility of results and methods are receiving increased attention, and the norms of research in many fields are changing (Nosek et al. 2015; Miguel et al. 2014; Marwick 2016).

There is strong interest in open, transparent, and reusable research in the geoscience community (Gil et al. 2016) and substantial progress toward open data has been made in the geosciences with the widespread use of data services of NASA, USGS, NOAA and community-built data portals such as OneGeology, EarthChem, RRUFF, PANGAEA, PaleoBioDB, and others (Kattge, Díaz, and Wirth 2014; Ma 2018). However, the use of open source software such as R (Pebesma, Nüst, and Bivand 2012), and sharing of scripted data analysis workflows with research publications is not yet widespread (Hutton et al. 2016). With this R package our goal is to make scripted and reproducible data analysis easy for open-system uranium-thorium dating. This will improve the transparency of geochronology research, and provide a more credible and robust foundation for scientific advancement (Hutton et al. 2016).

To enable re-use of our materials and improve reproducibility and transparency, all the results and visualisations in this paper can be reproduced using the RMarkdown vignette document included with the UThwgl package. We have archived these files at <http://doi.org/10.17605/OSF.IO/D5P7S> to ensure long-term accessibility. Our code is released under the MIT licence, our data as CC-0, and our figures as CC-BY, to enable maximum re-use (for more details, see Marwick 2016).

Methods

For U-Th dating, two types of analysis are possible: bulk or in-situ. For bulk analysis, a fraction of the samples is dissolved and the solution processed through ion exchange chromatography to separate U and Th (e.g. Luo et al. 1997). Each element is then analysed separately for their isotope ratios by mass spectrometry. For in-situ analysis, laser ablation is commonly used (Eggins et al. 2005). In this case, a laser with a spot size ranging from a few μm to several hundreds of μm produces an aerosol which is carried using a gas (helium or preferably a mixture of helium and nitrogen; Eggins, Kinsley, and Shelley (1998)). While laser ablation offers a better spatial resolution and is less time consuming than bulk analysis, the precision of the data is inferior because of the much smaller amount of material sampled.

Uranium and thorium isotope ratios are then analysed by multi-collector inductively-coupled plasma mass spectrometry (e.g. Luo et al. (1997); although bulk analysis can also be performed by thermal ionisation mass spectrometry).



Figure 1: Modern human femur (132A/LB/27D/03) from Liang Bua, Flores, Indonesia. Two analysis transects can be seen. For a given transect, the outer and inner surface of the bone are given 1 and -1 reference coordinates, and the position of each analysis is calculated accordingly. Modified from Sutikna et al. (2016).

90 A plasma ionise U and Th atoms, their isotopes are separated through a mag-
 91 netic field and each collected in a different collector. If using laser ablation, it is
 92 best to have two ion counters so ^{230}Th and ^{234}U can be collected simultaneously.

93 *Closed-system dating*

94 Pending closed-system behaviour can be assessed, it is possible to derive an
 95 age for each U-Th analysis. The closed-system function `csUTh()` requires that
 96 for each analysis to yield an age, $(^{234}\text{U}/^{238}\text{U})$, $(^{230}\text{Th}/^{238}\text{U})$ and $(^{232}\text{Th}/^{238}\text{U})$
 97 activity ratios are measured (parentheses denote activity ratios throughout this
 98 article). The $(^{232}\text{Th}/^{238}\text{U})$ activity ratio is required for detrital correction (note
 99 it is needed to use `csUTh()` whether the detrital correction is performed or not).

100 *Open-system dating*

101 Data required for the DAD model are $(^{230}\text{Th}/^{238}\text{U})$ and $(^{234}\text{U}/^{238}\text{U})$ activity
 102 ratios collected along a transect perpendicular to the surface of the tooth or bone.
 103 Sampling for analysis can be done by micro-drilling or laser ablation.

104 The distance of each analysis location from the inner and outer surfaces of
 105 the bones, for instance, needs to be recorded. One surface is given a coordinate
 106 of 1 and the other one -1, thus coordinates of analyses take values in between
 107 (Figure 1).

108 Working with the package

109 We provide three methods for using this package to suit different levels of
110 familiarity with the R programming language. The simplest way to use the pack-
111 age is our web applications, online at <https://ben-marwick.shinyapps.io/csUTh/>
112 and <https://ben-marwick.shinyapps.io/osUTh/> (Figure 2). Using the web ap-
113 plication requires no familiarity with R. To use the web application we upload
114 a CSV file, then click through a series of tabs to inspect the data, adjust the
115 model parameters, run the model, and inspect the output. The interface is
116 mouse-driven and requires no programming. In the web application we upload
117 the data file on the *Load the data* tab, set parameters from the *Set model pa-*
118 *rameters* tab, run the model by clicking the button *Run Simulation* on the same
119 tab, and observe the results on the *Visualise the model* and *Inspect the model*
120 tabs. We can change the parameters and re-run the model by click the button
121 *Run Simulation*. Once done, close the window.

122 The second way to use the package is with Binder, a browser-based instance
123 of R and RStudio that includes our package ready to work with. Binder is a
124 server technology that turns computational material, such as an R package, into
125 interactive computational environments in the cloud. Using Binder requires a
126 novice level of familiarity with R, for example to use the code in this paper and
127 adapt it to work with a different CSV file. Because Binder provides a complete
128 R environment, custom R code can be written during a Binder instance to
129 further explore the model’s output in the browser. These two methods, the
130 web application and Binder, do not require any software to be downloaded and
131 installed on the user’s computer, all computation occurs in the browser. The
132 web application and Binder are suitable for getting a quick start on working
133 with the package, but they require a connection to the internet, and they have
134 limited memory and compute time available per instance.

135 The third method is to download and install the package locally to the user’s
136 computer, and work with it in the user’s local installation of R and RStudio.
137 This method requires some familiarity with R, but gives the most flexibility
138 when working with the model because we are not limited by the memory and
139 compute time of the cloud services. Our recommendation is to use Binder or a
140 local installation of UThwgl because then the user can save an R script file that
141 includes the name of the input file, the specific parameters used to generate the
142 model output, and any downstream processing and visualisation. This script file
143 and the CSV file can then be archived in a data repository to ensure long-term
144 accessibility for other researchers. In the following sections we demonstrate the
145 use of UThwgl with a local installation of R and RStudio.

146 Installing and attaching the package

147 First the user will need to download and install R, and we also recommend
148 downloading and installing RStudio. To run the model, start **RStudio** and

A UThwgl::osUth : compute open-system Uranium-Thorium ages using the diffusion-adsorption-decay (DAD) model

Load the data Inspect the data Set model parameters

Visualise the model Inspect the model

Before uploading, check that your CSV file contains columns with these names:

- idAD.position**: coordinates of the ($^{234}\text{U}/^{238}\text{U}$) analyses, which take values between -1 and 1 (0: center of the bone; -1 and 1: inner and outer surfaces of the bone, respectively)
- U234_U238_CORR**: activity ratios
- U234_U238_CORR_1m2SE**: the 2 sigma errors of the activity ratios
- idAD.position.1**: coordinates of the ($^{230}\text{Th}/^{232}\text{Th}$) analyses, which take values between -1 and 1 (can be the same or different values from those of the ($^{234}\text{U}/^{238}\text{U}$) analyses)
- Th230_U238_CORR**: activity ratios
- Th230_U238_CORR_1m2SE**: the 2 sigma errors of the activity ratios
- U_ppm**: calculated uranium concentrations (in ppm)
- U_ppm_1m2SE**: the 2 sigma errors of the uranium concentrations

Choose CSV file

Browse... **Hobbit_1987T_for_idAD.csv**

Upload complete

Go to inspect the data

C UThwgl::osUth : compute open-system Uranium-Thorium ages using the diffusion-adsorption-decay (DAD) model

Load the data Inspect the data Set model parameters

Visualise the model Inspect the model

Number of iterations: 100

Value of squared sum: 0.01

Thickness of sample (cm): 5.35

Uranium concentration at the sample surface (ppm): 25

Min U diffusion coefficient: 0.000000000001

Max U diffusion coefficient: 0.000000000001

Run simulation and visualise the output

E UThwgl::osUth : compute open-system Uranium-Thorium ages using the diffusion-adsorption-decay (DAD) model

Load the data Inspect the data Set model parameters

Visualise the model Inspect the model

| Age (ka) | Age 67% quantile (ka) | Age 33% quantile (ka) | U234_U238_0 | U234_U238_0 67% quantile | U234_U238_0 33% quantile |
|----------|-----------------------|-----------------------|-------------|--------------------------|--------------------------|
| 6.82 | 0.58 | 0.53 | 1.27 | 0.01 | 0.00 |

| diff | T_final | K_final | T_sol |
|----------|---------|---------|---------|
| 695.89 | 6817.35 | 0.00 | 7492.41 |
| -1149.35 | 6817.35 | 0.00 | 5647.17 |
| 1898.93 | 6817.35 | 0.00 | 8695.46 |
| -1123.74 | 6817.35 | 0.00 | 5672.78 |
| 1370.91 | 6817.35 | 0.00 | 8167.43 |
| -1634.21 | 6817.35 | 0.00 | 5162.31 |
| -20.83 | 6817.35 | 0.00 | 6775.70 |
| 1051.79 | 6817.35 | 0.00 | 7848.31 |
| -1489.97 | 6817.35 | 0.00 | 5333.55 |

B UThwgl::osUth : compute open-system Uranium-Thorium ages using the diffusion-adsorption-decay (DAD) model

Load the data Inspect the data Set model parameters

Visualise the model Inspect the model

Here is the raw data from the CSV file

Show 10 entries

| | idAD.position | U234_U238_CORR | U234_U238_CORR_1m2SE | idAD.position.1 |
|----|---------------|----------------|----------------------|-----------------|
| 1 | -0.95588237 | 1.2696216 | 0.00421 | -0.95588237 |
| 2 | -0.85681117 | 1.2729341 | 0.00424 | -0.85681117 |
| 3 | -0.75773996 | 1.2654235 | 0.00372 | -0.75773996 |
| 4 | -0.65866876 | 1.2673451 | 0.00454 | -0.65866876 |
| 5 | -0.55959755 | 1.2691554 | 0.00291 | -0.55959755 |
| 6 | -0.46052632 | 1.2655151 | 0.00284 | -0.46052632 |
| 7 | -0.36145511 | 1.266979 | 0.00255 | -0.36145511 |
| 8 | -0.26238391 | 1.2760185 | 0.00231 | -0.26238391 |
| 9 | -0.16331269 | 1.265514 | 0.00228 | -0.16331269 |
| 10 | -0.0642 | 1.2766815 | 0.0021 | -0.0642 |

Showing 1 to 10 of 20 entries

Go to set the model parameters

D UThwgl::osUth : compute open-system Uranium-Thorium ages using the diffusion-adsorption-decay (DAD) model

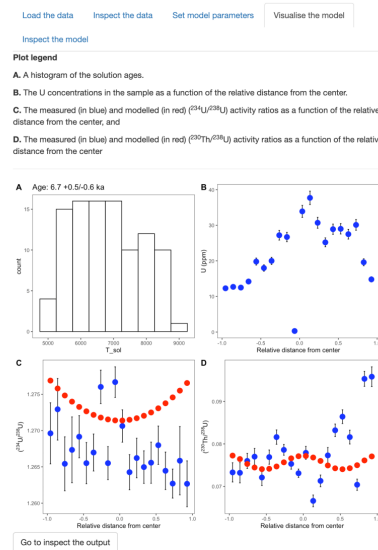


Figure 2: Screenshots of the web application for using the UThwgl package. A: Upload a CSV file of the data to model, B: Inspect a table of the uploaded data. C: Set the model parameters and run the model. D: Inspect visualisations of the model's output. E: Inspect and download the numeric output from the model.

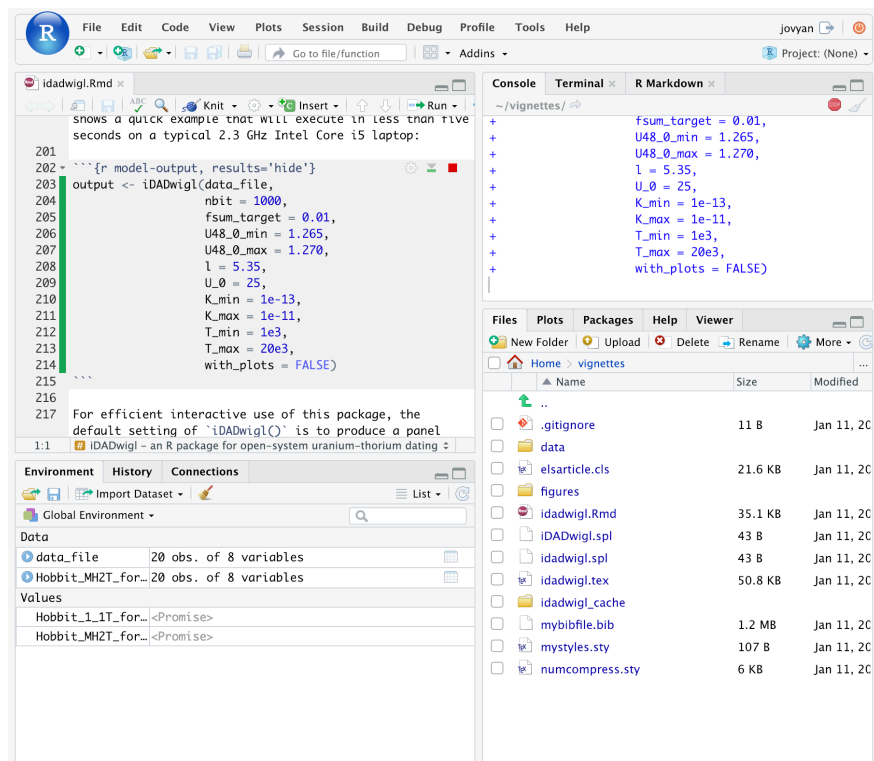


Figure 3: Screenshot of Binder running R and RStudio in a web browser window.

149 install the package from GitHub. There are many ways to do this, one simple
150 method is shown in the line below. This only needs to be done once per
151 computer.

```
if(!require("remotes")) install.packages("remotes")
remotes::install_github("tonydoss/UThwgl")
```

152 For routine data analysis, R scripts need to contain the following line to
153 attach the package to the current working environment. This line needs to be
154 run at the start of each analysis:

```
# attach the package
library(UThwgl)
```


155 Closed-system U-Th dating

156 *Input data format*

157 Our package provides the function `csUTh()` for closed-system U-Th dating.
158 Data for this function needs to be in a data frame (a form of table in R) with
159 the following column names:

- 160 • `Sample_ID`
- 161 • `U234_U238_CORR`
- 162 • `U234_U238_CORR_Int2SE`
- 163 • `Th230_U238_CORR`
- 164 • `Th230_U238_CORR_Int2SE`
- 165 • `Th232_U238_CORR`
- 166 • `Th232_U238_CORR_Int2SE`

167 To help with preparing data for input into our function, we have included an
168 example of an input file, taken from Pan et al. (2018). Inspecting the included
169 data sets will be helpful for understanding how to prepare new data to prepare
170 for use with this package. After attaching the package, we can access the built-in
171 datasets with the `data()` function, like this:

```
# access the data included in the UThwigl package
data("Pan2018")
```

172 This will make the built-in data available in the R environment to inspect
173 and explore how to use the `csUTh()` function. To use new data with this pack-
174 age, the user needs to import a CSV or Excel file with the U-Th data into the
175 R environment. This can be done using a generic function such as `read.csv`
176 or `read_excel` from the `readxl` package (Wickham and Bryan 2018). Before
177 reading in the data file, the user needs to set the working directory to the folder
178 containing the data file. This can be done in RStudio using the menu item
179 ‘Session’ > ‘Set Working Directory’ > ‘To Source File Location’. Alternatively,
180 the working directory can be defined interactively at the R prompt in the Con-
181 sole panel using `setwd()`. However, we do not recommend including `setwd()`
182 in script files because it is bad for reproducibility, since the path to one user’s
183 working directory will not exist on another user’s computer.

184 To download the built-in data to the user’s computer so it can be inspected
185 and modified in a spreadsheet program, use `write.csv()`

```
# download the data included in the package
write.csv(Pan2018, "Pan2018.csv")
```

186 The code chunk below shows how to read one of the CSV files included in the
187 package into the R environment. We assume that the user’s working directory
188 contains a directory called `data` and the CSV file is in this `data` directory, and
189 so the data can be imported as follows:

```
# read in one of the example CSV files included in the package
input_data_cs <-
  read.csv('data/Pan2018.csv')
```

Table 1 shows the data contained in the Pan2018.csv file included in the package.

| Sample_ID | U234_U238_CORR | U234_U238_CORR_Int2SE | Th230_U238_CORR | Th230_U238_CORR_Int2SE | Th232_U238_CORR | Th232_U238_CORR_Int2SE |
|-----------|----------------|-----------------------|-----------------|------------------------|-----------------|------------------------|
| YP002A | 1.150 | 0.005 | 0.794 | 0.007 | 0.010 | 0.00005 |
| YP002B | 1.120 | 0.004 | 0.788 | 0.006 | 0.004 | 0.00002 |
| YP003-1_1 | 1.125 | 0.004 | 0.752 | 0.010 | 0.000 | 0.00001 |
| YP003-1_2 | 1.113 | 0.007 | 0.761 | 0.011 | 0.000 | 0.00000 |
| YP003-1_3 | 1.122 | 0.005 | 0.748 | 0.008 | 0.001 | 0.00001 |
| YP003-1_4 | 1.122 | 0.005 | 0.726 | 0.007 | 0.001 | 0.00001 |
| YP003-1_5 | 1.119 | 0.006 | 0.757 | 0.006 | 0.002 | 0.00001 |
| YP002-1_1 | 1.129 | 0.006 | 0.722 | 0.008 | 0.001 | 0.00001 |
| YP002-1_2 | 1.137 | 0.005 | 0.767 | 0.008 | 0.001 | 0.00001 |
| YP002-1_3 | 1.118 | 0.008 | 0.739 | 0.009 | 0.002 | 0.00002 |
| YP002-1_4 | 1.114 | 0.006 | 0.749 | 0.008 | 0.003 | 0.00003 |
| YP002-1_5 | 1.105 | 0.007 | 0.764 | 0.011 | 0.003 | 0.00004 |

Table 1: Data contained in the example CSV file Pan2018.csv included in the package

The columns Sample_ID, U234_U238_CORR, U234_U238_CORR_Int2SE, Th230_U238_CORR, Th230_U238_CORR_Int2SE, Th232_U238_CORR and Th232_U238_CORR_Int2SE must be present in the input data frame with these exact names for the model to function. The csUTh() function will check if the input data frame has these columns, and will stop with an error message if it does not find these columns. The names() function can be used to update column names of a data frame to ensure they match the names that the model function requires. Alternatively the user can edit the column names in a spreadsheet program such as Microsoft Excel. The order of the columns in the data frame is not important.

Columns U234_U238_CORR and U234_U238_CORR_Int2SE are the ($^{234}\text{U}/^{238}\text{U}$) activity ratios and their 2σ errors. Columns Th230_U238_CORR and Th230_U238_CORR_Int2SE are the ($^{230}\text{Th}/^{238}\text{U}$) activity ratios and their 2σ errors. Columns Th232_U238_CORR

204 and `Th232_U238_CORR_Int2SE` are the ($^{232}\text{Th}/^{238}\text{U}$) activity ratios and their 2σ
 205 errors.

206 *Details of the input parameters of closed-system analysis*

207 `sample_name` is the name of the sample to calculate closed-system ages for.
 208 The function will partially match by sample prefix. For example in Table 1 one
 209 sample is indicated by the Sample ID ‘YP003’. If the user inputs ‘YP003’ for
 210 the `sample_name`, then this will match rows where the Sample ID is ‘YP003-1’,
 211 ‘YP003-2’, ‘YP003-3’, and so on.

212 `nbitchoice` is the number of iterations in the model. Recommended to have
 213 at least 100. `detcorrectionchoice` is a parameter for choosing whether or not
 214 to apply a detrital correction to the calculation.

215 `R28det` (0.8) and `R28det_err` (0.08) are the values for the ($^{232}\text{Th}/^{238}\text{U}$)
 216 activity ratio of the detritus and its standard error (default values in paren-
 217 theses). Similarly, `R08det` (1) and `R08det_err` (0.05) are the values for the
 218 ($^{230}\text{Th}/^{238}\text{U}$) activity ratio of the detritus and its standard error, and `R48det`
 219 (1) and `R48det_err` (0.02) are the corresponding values for ($^{234}\text{U}/^{238}\text{U}$) activity
 220 ratio of the detritus.

221 *How to run the model*

222 Assuming that the package is attached with `library(UThwig1)`, as shown
 223 above, and the data have been imported to the working environment as noted
 224 above, run `csUTh()`, specifying the input data frame and the input parameters
 225 as described above. The code block below shows a typical example that will
 226 execute in less than five seconds on a typical 2.3 GHz Intel Core i5 laptop:

```
# Solve for sample YP003 in-situ analyses
output_cs <-
  csUTh(
    input_data_cs,
    sample_name = 'YP003',
    nbitchoice = 100,
    detcorrectionchoice = TRUE,
    keepfiltereddata = FALSE,
    print_summary = TRUE,
    with_plots = TRUE,
    save_plots = FALSE,
    save_output = FALSE
  )
```

227 For efficient interactive use of this package, the default setting of `csUTh()` is
 228 to produce a panel plot as seen in Figure 4. The setting `with_plots = FALSE`
 229 prevents plots from being generated which is more useful when the function is
 230 part of a longer sequence of code. The function runs faster when not producing
 231 pots, which is helpful when replicating many runs. The setting `save_output`
 232 `= TRUE` will save a csv file to the current working directory so the output data

233 can be used in other contexts. The csv file that is created when `save_output`
 234 `= TRUE` will be given a name that includes a date and time stamp so that the
 235 output of each time the function is run can be saved to a unique file.

236 When run on the R console, this function will print a confirmation that the
 237 input data frame has the required columns. If `print_summary` is set to `TRUE`,
 238 it will also the resulting mean age value of several analyses on a single sample,
 239 with an error reported as 2 Standard Error, for example:

```
240 All required columns are present in the input data
241 [1] "Mean age: 117.1 +/- 3.7 ka"
```

242 `print_summary` should be set to `FALSE` if ages computed are not for analyses
 243 of the same sample, since this mean age would be meaningless.

244 *Inspecting and visualizing the models' output*

245 The function returns a data frame with the age, error and summary output
 246 for each measurement, as shown in Table 2. This includes calculated ages (with
 247 or without detrital correction, depending how `detcorrectionchoice` was set),
 248 initial ($^{234}\text{U}/^{238}\text{U}$) activity ratios, along with their uncertainties.

| Sample ID | Age (ka) | Age 2se | ($^{234}\text{U}/^{238}\text{U}$)i | Ratio 2se |
|-----------|----------|---------|--------------------------------------|-----------|
| YP003-1_1 | 117.006 | 0.3440 | 1.1740 | 0.0010 |
| YP003-1_2 | 121.569 | 0.3810 | 1.1600 | 0.0010 |
| YP003-1_3 | 116.299 | 0.2810 | 1.1710 | 0.0010 |
| YP003-1_4 | 110.713 | 0.2520 | 1.1660 | 0.0010 |
| YP003-1_5 | 119.542 | 0.2540 | 1.1660 | 0.0010 |

Table 2: Output produced by the `csUTh` function used with data from Pan et al. 2018

249 The plots produced by the `csUTh()` function are stored as list objects in the
 250 output from the function. We can show the plots by accessing the list like this:

```
output_cs$plots
```

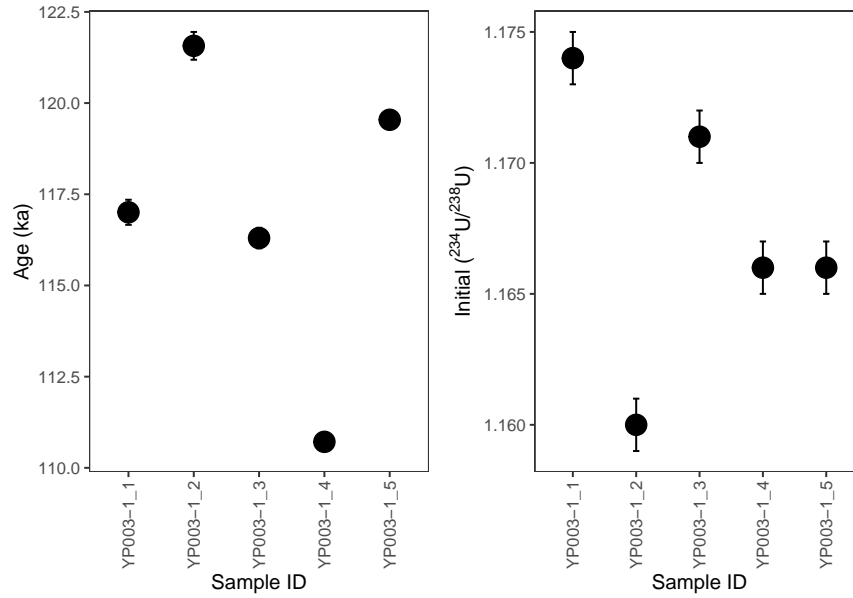


Figure 4: Example of the visualisations produced by the `csUTh()` function, using the demonstration run described above, and five in-situ analyses by laser ablation of coral sample YP003. A: closed-system ages and B: initial ($^{234}\text{U}/^{238}\text{U}$) activity ratios for each sample analysis

Open-system U-Th dating

Input data format

For open-system U-Th dating we provide the function `osUTh()`, which requires a data frame with the following column names:

- `iDAD.position`
- `U234_U238_CORR`
- `U234_U238_CORR_Int2SE`
- `iDAD.position.1`
- `Th230_U238_CORR`
- `Th230_U238_CORR_Int2SE`
- `U_ppm`
- `U_ppm_Int2SE`

We have included two examples of input files. After attaching the package, we can access the built-in datasets with the `data()` function, like this:

```
# access the data included in the UThwigl package
data("Hobbit_1_1T_for_iDAD")
data("Hobbit_MH2T_for_iDAD")
```

As above, these datasets can be downloaded from the package with `write.csv()`:

```
# download the data included in the package
write.csv(Hobbit_1_1T_for_iDAD, "Hobbit_1_1T_for_iDAD.csv")
write.csv(Hobbit_MH2T_for_iDAD, "HHobbit_MH2T_for_iDAD.csv")
```

266 The code chunk below shows how to read one of the CSV files included
267 in the package into the R environment. As above, we assume that the user's
268 working directory contains a directory called `data` and the CSV file is in this
269 `data` directory, and so the data can be imported as follows:

```
# read in one of the example CSV files included in the package
input_data_os <-
  read.csv('data/Hobbit_MH2T_for_iDAD.csv')
```

Table 3 shows the data contained in the `Hobbit_MH2T_for_iDAD.csv` file included in the package

| iDAD.position | U234_U238_CORR | U234_U238_CORR_Int2SE | iDAD.position.1 | Th230_U238_CORR | Th230_U238_CORR_Int2SE | U_ppm | U_ppm_Int2SE |
|---------------|----------------|-----------------------|-----------------|-----------------|------------------------|-------|--------------|
| -0.956 | 1.270 | 0.004 | -0.956 | 0.073 | 0.002 | 12.3 | 0.6 |
| -0.857 | 1.273 | 0.004 | -0.857 | 0.073 | 0.002 | 12.7 | 0.6 |
| -0.758 | 1.265 | 0.004 | -0.758 | 0.076 | 0.002 | 12.5 | 0.6 |
| -0.659 | 1.267 | 0.005 | -0.659 | 0.077 | 0.002 | 14.2 | 0.7 |
| -0.560 | 1.269 | 0.003 | -0.560 | 0.072 | 0.002 | 19.8 | 1.0 |
| -0.461 | 1.266 | 0.003 | -0.461 | 0.077 | 0.002 | 18.0 | 0.9 |
| -0.361 | 1.267 | 0.003 | -0.361 | 0.082 | 0.002 | 20.0 | 1.0 |
| -0.262 | 1.276 | 0.002 | -0.262 | 0.079 | 0.001 | 27.2 | 1.4 |
| -0.163 | 1.266 | 0.002 | -0.163 | 0.075 | 0.001 | 26.7 | 1.3 |
| -0.064 | 1.277 | 0.002 | -0.064 | 0.073 | 0.001 | 0.3 | 0.0 |
| 0.035 | 1.271 | 0.002 | 0.035 | 0.078 | 0.002 | 33.9 | 1.7 |
| 0.134 | 1.264 | 0.002 | 0.134 | 0.067 | 0.001 | 37.7 | 1.9 |
| 0.233 | 1.266 | 0.003 | 0.233 | 0.071 | 0.001 | 30.7 | 1.5 |
| 0.332 | 1.265 | 0.002 | 0.332 | 0.077 | 0.002 | 25.2 | 1.3 |
| 0.431 | 1.266 | 0.003 | 0.431 | 0.083 | 0.001 | 28.9 | 1.4 |
| 0.530 | 1.268 | 0.003 | 0.530 | 0.086 | 0.002 | 29.0 | 1.4 |
| 0.629 | 1.264 | 0.003 | 0.629 | 0.082 | 0.002 | 27.5 | 1.4 |
| 0.728 | 1.263 | 0.002 | 0.728 | 0.070 | 0.001 | 30.1 | 1.5 |
| 0.827 | 1.266 | 0.005 | 0.827 | 0.095 | 0.002 | 19.6 | 1.0 |
| 0.926 | 1.263 | 0.003 | 0.926 | 0.096 | 0.002 | 14.8 | 0.7 |

Table 3: Data contained in the example CSV file `Hobbit_MH2T_for_iDAD.csv` included in the package

As for the closed-system function, the columns `iDAD.position`, `U234_U238_CORR`, `U234_U238_CORR_Int2SE`, `Th230_U238_CORR` and `Th230_U238_CORR_Int2SE` must be present in the input data frame with these exact names for the model to function. The `osUTh()` function will check if the input data frame has these columns, and will stop with an error message if it does not find these columns.

The `iDAD.position` column corresponds to the coordinates of the ($^{234}\text{U}/^{238}\text{U}$) analyses, which as indicated above take values between -1 and 1 (Figure 1). The second `iDAD.position.1` column is used if the coordinates of the ($^{230}\text{Th}/^{238}\text{U}$)

analyses are different from those of the ($^{234}\text{U}/^{238}\text{U}$) analyses.

Columns `U_ppm` and `U_ppm_Int2SE` are the calculated uranium concentrations (in ppm) and their 2σ errors. Uranium concentrations are not necessary for the model but needed to display the U concentration profile in a figure.

Details of the input parameters of open-system analysis

Our key function, `osUTh()` has several arguments that need to be set before meaningful results can be obtained:

`nbit` is the number of iterations. For the first run, set to 1.

`fsum_target` is the sum of the squared differences between the calculated and observed activity ratios. Give it a low value to start with (e.g. 0.01). If script takes too long, try a higher value for `fsum_target`.

`U48_0_min` and `U48_0_max` are the minimum and maximum values allowed for the ($^{234}\text{U}/^{238}\text{U}$) activity ratio at the surface of the sample. Since ($^{234}\text{U}/^{238}\text{U}$) does not vary greatly over the time period generally studied, the values measured near the surface of the sample can be used as a guide. These values can be adjusted if the model fit to the data is not optimal. For `Hobbit_1-1T` they are taken to be 1.360 and 1.375, and for `Hobbit_MH2T`, 1.265 and 1.270, respectively.

`l` is the thickness of the sample in centimeters. For `Hobbit_1-1T` it is 3.5 cm, for `Hobbit_MH2T` it is 5.35 cm

`U_0` is the uranium concentration at the surface in ppm. This value does not significantly affect the model results and values from analyses near either surface of the sample can be used as a guide. For `Hobbit_1-1T` it is taken to be 15 ppm; for `Hobbit_MH2T`, 25 ppm.

`K_min` and `K_max` are the minimum and maximum values allowed for the uranium diffusion coefficient (in cm^2/s). Values between 10^{-13} and 10^{-11} cm^2/s are generally appropriate.

`T_min` and `T_max` are the minimum and maximum values for the age of the specimen (yr). If there is no estimated knowledge of the sample age, the range of values can be 1,000 to 500,000 yr and adjusted later. For `Hobbit_1-1T`, in the final model run, they are taken to be 50,000 and 100,000 yr, and for `Hobbit_MH2T`, 1,000 and 20,000 yr, respectively.

After setting the U480 maximum and minimum values, run the function and adjust these min and max values by looking at the calculated `U48_0_final`, `K_final`, and `T_final`. Adjust `T_min` and `T_max` using first estimates of the age. As we iterate, increase the `nbit` value to reduce the error.

How to run the model

Attach the package as shown above and then run `osUTh()`, specifying the input data frame and the input parameters as described above. The code block below shows a quick example that will execute in less than five seconds on a typical 2.3 GHz Intel Core i5 laptop:


```

output_os <- osUTh(input_data_os,
                    nbit = 1000,
                    fsum_target = 0.01,
                    U48_0_min = 1.265,
                    U48_0_max = 1.270,
                    l = 5.35,
                    U_0 = 25,
                    K_min = 1e-13,
                    K_max = 1e-11,
                    T_min = 1e3,
                    T_max = 20e3,
                    with_plots = TRUE,
                    save_plots = FALSE,
                    save_output = FALSE)

```

321 The default setting of `osUTh()` is to produce a panel plot as seen in Figure
 322 5(Figure 5. The setting `with_plots = FALSE` prevents plots from being gen-
 323 erated which is more useful when the function is part of a longer sequence of
 324 code. The function runs faster when not producing pots, which is helpful when
 325 replicating many runs.

326 Similar to the `csUTh()` function, when `osUTh()` is run on the R console, it
 327 will print a confirmation that the input data frame has the required columns,
 328 and print the resulting age value with an error reported as the 67% and 33%
 329 quantiles, for example:

```

330 All required columns are present in the input data
331 [1] "Age: 7 +0.6/-0.7 ka"

```

332 The model computes a Monte Carlo simulation where age of the sample,
 333 U diffusion coefficient and ($^{234}\text{U}/^{238}\text{U}$) ratio at the surface of the sample are
 334 taken randomly within the range of values allowed. Results are only kept if the
 335 calculated sum of the squared differences between the calculated and observed
 336 activity ratios is less than the value set in `fsum_target`. If this is the case,
 337 the calculated ratios and the set of solutions for age of the sample, U diffusion
 338 coefficient and ($^{234}\text{U}/^{238}\text{U}$) ratio at the surface of the sample are saved. The
 339 model stops once the number of sets of solutions reaches `nbit`.

340 The final calculated age `T_final` (in yr), U diffusion coefficient `K_final` (in
 341 cm^2/s) and ($^{234}\text{U}/^{238}\text{U}$) ratio at the surface of the sample `U48_0_final` are the
 342 set of solutions where the solution age is the closest to the median age of the
 343 population of solutions. The uncertainty on each output paramter is calculated
 344 as the 67% and 33% quantiles of the population of solution sets.

345 In a typical analysis the user will explore the model fit by first running the
 346 model with a single iteration `nbit` and a small value for `fsum_target`, and then
 347 changing the range of allowed values for the ($^{234}\text{U}/^{238}\text{U}$) ratio at the surface
 348 and the age of the sample. Once the user has obtained a satisfying fit (by visual
 349 inspection of the produced figures), they would increase `nbit` to a higher value

(e.g. 1000) and run the model one last time. We provide an example of a typical analysis analysis below.

Inspecting the models' output

`T_final`, `K_final` and `U48_0_final` are included in the model's output, along with their uncertainties. The function also includes a one-row data frame summarising the age:

| Age (ka) | Age 67% quantile (ka) | Age 33% quantile (ka) | U234_U238_0 | U234_U238_0 67% quantile | U234_U238_0 33% quantile |
|----------|-----------------------|-----------------------|-------------|--------------------------|--------------------------|
| 6.87 | 0.63 | 0.63 | 1.2679 | 0.0021 | 0.0029 |

Table 4: Summary table of the computed age and error values

The last item in the output is a copy of the input data with two additional columns, the calculated activity ratios, ($^{234}\text{U}/^{238}\text{U}$) and ($^{230}\text{Th}/^{238}\text{U}$), for each measurement location on the sample.

Visualising the models' output

`osUTh()` returns several figures useful for visualisation of the model results along with the data:

1. a histogram of the solution ages (Figure 5 A)
2. the U concentrations in the sample as a function of the relative distance from the center (Figure 5 B)
3. the measured (in blue) and modelled (in red) ($^{234}\text{U}/^{238}\text{U}$) activity ratios as a function of the relative distance from the center (Figure 5 C), and
4. the measured (in blue) and modelled (in red) ($^{230}\text{Th}/^{238}\text{U}$) activity ratios as a function of the relative distance from the center (Figure 5 D).

We can show the plots produced by `osUTh()` by accessing the list like this:

```
output_os$plots
```

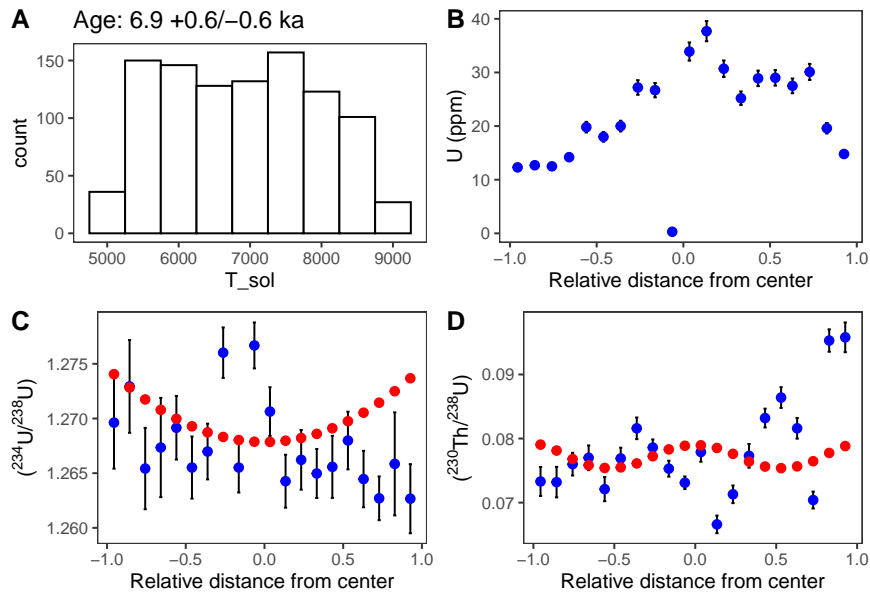


Figure 5: Example of the visualisations produced by the `osUTh()` function, using the demonstration run described above. A: Histogram of the solution ages, B: Uranium concentration profile for transect 2 of modern human femur 132A/LB/27D/03. C: Calculated (red) and observed (blue) $(^{234}\text{U}/^{238}\text{U})$ activity ratios for transect 2 of modern human femur 132A/LB/27D/03. D: Calculated (red) and observed (blue) $(^{230}\text{Th}/^{238}\text{U})$ activity ratios for transect 2 of modern human femur 132A/LB/27D/03.

| iDAD.position | U234_U238_CORR | U234_U238_CORR_Int2SE | iDAD.position.1 | Th230_U238_CORR | Th230_U238_CORR_Int2SE | U_ppm | U_ppm_Int2SE | U234_U238_CALC | Th230_U238_CALC |
|---------------|----------------|-----------------------|-----------------|-----------------|------------------------|-------|--------------|----------------|-----------------|
| -0.956 | 1.270 | 0.004 | -0.956 | 0.073 | 0.002 | 12.3 | 0.6 | 1.274 | 0.079 |
| -0.857 | 1.273 | 0.004 | -0.857 | 0.073 | 0.002 | 12.7 | 0.6 | 1.273 | 0.078 |
| -0.758 | 1.265 | 0.004 | -0.758 | 0.076 | 0.002 | 12.5 | 0.6 | 1.272 | 0.077 |
| -0.659 | 1.267 | 0.005 | -0.659 | 0.077 | 0.002 | 14.2 | 0.7 | 1.271 | 0.076 |
| -0.560 | 1.269 | 0.003 | -0.560 | 0.072 | 0.002 | 19.8 | 1.0 | 1.270 | 0.075 |
| -0.461 | 1.266 | 0.003 | -0.461 | 0.077 | 0.002 | 18.0 | 0.9 | 1.269 | 0.076 |
| -0.361 | 1.267 | 0.003 | -0.361 | 0.082 | 0.002 | 20.0 | 1.0 | 1.269 | 0.076 |
| -0.262 | 1.276 | 0.002 | -0.262 | 0.079 | 0.001 | 27.2 | 1.4 | 1.268 | 0.077 |
| -0.163 | 1.266 | 0.002 | -0.163 | 0.075 | 0.001 | 26.7 | 1.3 | 1.268 | 0.078 |
| -0.064 | 1.277 | 0.002 | -0.064 | 0.073 | 0.001 | 0.3 | 0.0 | 1.268 | 0.079 |
| 0.035 | 1.271 | 0.002 | 0.035 | 0.078 | 0.002 | 33.9 | 1.7 | 1.268 | 0.079 |
| 0.134 | 1.264 | 0.002 | 0.134 | 0.067 | 0.001 | 37.7 | 1.9 | 1.268 | 0.079 |
| 0.233 | 1.266 | 0.003 | 0.233 | 0.071 | 0.001 | 30.7 | 1.5 | 1.268 | 0.078 |
| 0.332 | 1.265 | 0.002 | 0.332 | 0.077 | 0.002 | 25.2 | 1.3 | 1.269 | 0.076 |
| 0.431 | 1.266 | 0.003 | 0.431 | 0.083 | 0.001 | 28.9 | 1.4 | 1.269 | 0.076 |
| 0.530 | 1.268 | 0.003 | 0.530 | 0.086 | 0.002 | 29.0 | 1.4 | 1.270 | 0.075 |
| 0.629 | 1.264 | 0.003 | 0.629 | 0.082 | 0.002 | 27.5 | 1.4 | 1.271 | 0.076 |
| 0.728 | 1.263 | 0.002 | 0.728 | 0.070 | 0.001 | 30.1 | 1.5 | 1.271 | 0.076 |
| 0.827 | 1.266 | 0.005 | 0.827 | 0.095 | 0.002 | 19.6 | 1.0 | 1.272 | 0.078 |
| 0.926 | 1.263 | 0.003 | 0.926 | 0.096 | 0.002 | 14.8 | 0.7 | 1.274 | 0.079 |

Table 5: Example of output table including the input data described above, and two new columns

370 Case studies

371 *Closed-system dating - Case study from Pan et al. 2018*

372 The package includes sample data from Marine Isotope Stage 5 corals from
373 Pan et al. (2018) (Table 1). Two *Plesiastrea versipora* coral samples were
374 analysed: YP002 and YP003. The first two rows in Table 1 are bulk analyses
375 while the rest are in-situ analyses produced by laser ablation (hence the lower
376 precision compared to the first two row). In Pan et al. (2018), closed-system
377 ages were calculated using IsoPlot 4.15 (K. R. Ludwig 2003). For bulk analyses,
378 Pan et al. (2018) reported detrital-corrected ages of 121.4 ± 2.4 ka and 127.3
379 ± 2.1 ka for YP002A and YP002B, respectively. For in-situ analyses, Pan et al.
380 (2018) reported mean detrital-corrected ages of five analyses for each sample:
381 117.5 ± 4.5 ka for YP002 and 115.0 ± 5.4 ka for YP003.

382 Here we solve the closed-system model for all samples by simply entering ‘YP’
383 against `sample_name` since all analyses in the table contain these two characters
384 in their `Sample_ID` column. `print_summary` is set to `FALSE` since we are solving
385 for different samples and a mean age would have no significance.

```
# Solve for all samples
output_cs_all <-
  csUTh(
    input_data_cs,
    sample_name = 'YP',
    nbitchoice = 100,
    detcorrectionchoice = TRUE,
    keepfiltereddata = FALSE,
    print_summary = FALSE,
    with_plots = TRUE,
    save_plots = FALSE
  )
```

386 We obtain detrital-corrected ages of 123.2 ± 0.2 ka and 128.1 ± 0.2 ka for
387 bulk analyses of YP002 and YP003, respectively. This is within error of values
388 reported in Pan et al. (2018).

389 In-situ analyses for YP003-1 were solved above and yielded a mean detrital-
390 corrected age for the five analyses of 117.1 ± 3.7 ka, within error of the value
391 reported in Pan et al. (2018). We can solve also for in-situ analyses of YP002-1
392 by setting `sample_name` to ‘YP002-1’ and `print_summary` to `TRUE`:

```
# Solve for YP002 in-situ analyses
output_cs_YP002insitu <-
  csUTh(
    input_data_cs,
    sample_name = 'YP002-1',
    nbitchoice = 100,
    detcorrectionchoice = TRUE,
```

```

keepfiltereddata = FALSE,
print_summary = TRUE,
with_plots = TRUE,
save_plots = FALSE
)

```

393 We obtain a mean detrital-corrected age for the five analyses of 117 ± 5.3
394 ka, also within error of the value reported in Pan et al. (2018).

395 *Open-system dating - Case study of two ages from Sutikna et al. 2016*

396 The package includes two sample data sets derived from Sutikna et al.
397 (2016) : “Hobbit_MH2T_for_iDAD.csv” is data from transect 2 for mod-
398 ern human femur 132A/LB/27D/03 (shown above in Table 3). “Hobbit_1-
399 1T_for_iDAD.csv” is data from transect 1 for *Homo floresiensis* ulna LB1/52
400 (Table 6). For the latter, six analyses were removed from the set as in Sutikna
401 et al. (2016).

| iDAD.position | U234_U238_CORR | U234_U238_CORR_Int2SE | iDAD.position.1 | Th230_U238_CORR | Th230_U238_CORR_Int2SE | U_ppm | U_ppm_Int2SE |
|---------------|----------------|-----------------------|-----------------|-----------------|------------------------|-------|--------------|
| -0.143 | 1.369 | 0.002 | -0.143 | 0.699 | 0.006 | 32.0 | 1.6 |
| 0.165 | 1.370 | 0.002 | 0.165 | 0.733 | 0.008 | 41.1 | 2.1 |
| 0.319 | 1.364 | 0.002 | 0.319 | 0.672 | 0.006 | 35.8 | 1.8 |
| 0.472 | 1.362 | 0.003 | 0.472 | 0.636 | 0.006 | 27.6 | 1.4 |
| 0.626 | 1.365 | 0.003 | 0.626 | 0.641 | 0.006 | 31.0 | 1.6 |
| 0.780 | 1.374 | 0.003 | 0.780 | 0.712 | 0.005 | 27.9 | 1.4 |

Table 6: Data contained in the example CSV file Hobbit_11T_for_iDAD.csv included in the package

402 *Age of the modern human remains from Sutikna et al. 2016*

403 For transect 2 of 132A/LB/27D/03, Sutikna et al. (2016) reported an age
404 of 7.4 ± 0.5 ka (thousand years before 2014). With UThwgl, we first run
405 the model with `nbit = 1`, `fsum_target = 0.05`, `U48_0_min` and `U48_0_max`
406 `= 1.25` and `1.3`, respectively, `1 = 5.35` cm, `U_0 = 25` ppm, `K_min` and `K_max`
407 `= 10-13` and `10-11` cm²/s, respectively, `T_min` and `T_max = 103` and `500x103`
408 yr, respectively. `U48_0_min` and `U48_0_max` are determined by considering the

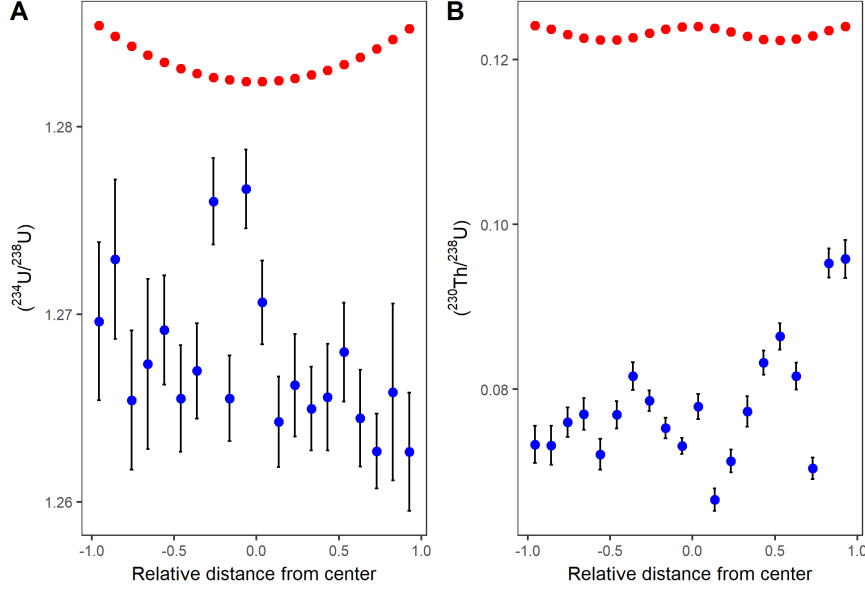


Figure 6: Results from the model's first run with the modern human femur. A: Calculated (red) and observed (blue) $(^{234}\text{U}/^{238}\text{U})$ activity ratios for transect 2 of modern human femur 132A/LB/27D/03. B: Calculated (red) and observed (blue) $(^{230}\text{Th}/^{238}\text{U})$ activity ratios for transect 2 of modern human femur 132A/LB/27D/03.

409 measured $(^{234}\text{U}/^{238}\text{U})$ values near the surfaces of the sample. T_{\min} and T_{\max}
 410 values were chosen such that no a priori knowledge of the age biases the results.

411 With this first run, we obtain an age of 11 ka. There is no calculated error
 412 on the age since there is only one iteration. In this case, we can see that the
 413 calculated $(^{234}\text{U}/^{238}\text{U})$ and $(^{230}\text{Th}/^{238}\text{U})$ ratios are too high (Figure 7). For the
 414 $(^{234}\text{U}/^{238}\text{U})$, it makes sense to thus use a lower value for $U48_0_{\max}$. Calculated
 415 $(^{230}\text{Th}/^{238}\text{U})$ ratios are too high compared to observed values suggest that the
 416 calculated age is too old (since this ratio increases with age). Thus, we should
 417 adjust T_{\max} accordingly.

418 Since the first run suggests a Holocene age for the sample, the measured
 419 $(^{234}\text{U}/^{238}\text{U})$ at the surfaces must be similar to the calculated values, thus the
 420 chosen values for the range above. Once $U48_0_{\min}$, $U48_0_{\max}$, T_{\min} and
 421 T_{\max} parameters have been adjusted, the model is run again. $fsum_target$
 422 can also be decreased to 0.01 in order to get a better fit and error, but it is at
 423 the expense of computing time. This operation is repeated until a satisfying
 424 fit is obtained (by visual inspection of the figures). Finally, the model is run
 425 once more, increasing the number of iterations to 1000 (or more). Following this
 426 method, we obtain an age of $6.2 \pm 1.2/-1.3$ ka (Figure 7). Note $(^{234}\text{U}/^{238}\text{U})$ and
 427 $(^{230}\text{Th}/^{238}\text{U})$ are still too high and low, respectively, so $U48_0_{\min}$, $U48_0_{\max}$,
 428 T_{\min} and T_{\max} parameters should be adjusted and the model run again.

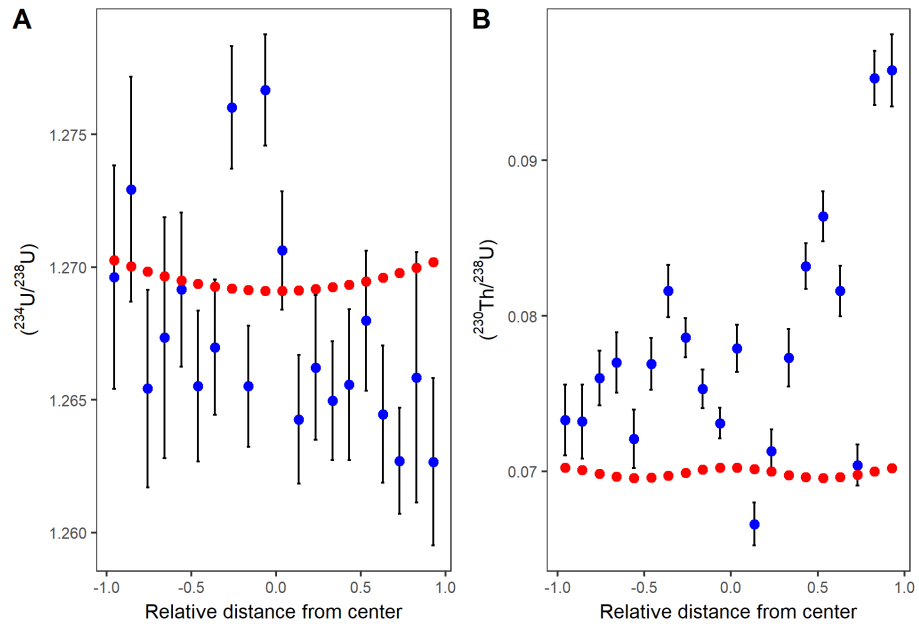


Figure 7: Results from the model's second run with the modern human femur. A: Calculated (red) and observed (blue) ($^{234}\text{U}/^{238}\text{U}$) activity ratios for transect 2 of modern human femur 132A/LB/27D/03. B: Calculated (red) and observed (blue) ($^{230}\text{Th}/^{238}\text{U}$) activity ratios for transect 2 of modern human femur 132A/LB/27D/03.

429 *Age of the Homo floresiensis remains from Sutikna et al. 2016*

430 For transect 1 of LB1/52, Sutikna et al. (2016) reported an age of 79.0 ± 3.7
431 ka. With osUth, using data in the file `Hobbit_1-1T_for_iDAD.csv` provided in
432 the package, and following the same method as above, we obtain an age of 75.4
433 $+1.0/-0.9$ ka (Figure 8).

434 Note that results and errors will vary slightly for each run since populations
435 are solution sets are randomly generated.

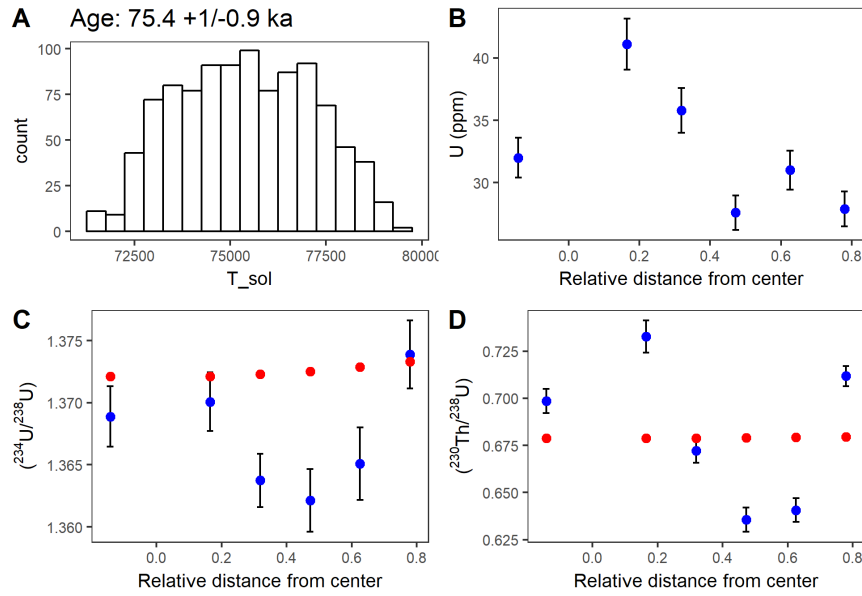


Figure 8: Results from running the model with *Homo floresiensis* ulna LB1/52 data from Sutikna et al. (2016). A: Histogram of the solution ages, B: Uranium concentration profile for transect 1 of *Homo floresiensis* ulna LB1/52. C: Calculated (red) and observed (blue) $(^{234}\text{U}/^{238}\text{U})$ activity ratios for transect 1 of *Homo floresiensis* ulna LB1/52. D: Calculated (red) and observed (blue) $(^{230}\text{Th}/^{238}\text{U})$ activity ratios for transect 1 of *Homo floresiensis* ulna LB1/52.

Conclusions

In this paper we have described `UThwig1`, an open source R package for computation of open-system U-Th ages. This helps to enable transparency, reproducibility, and flexibility of the analytical workflow for computing U-Th ages. The examples above show that results from our model are within error of previously published ages.

References

- Camerer, Colin F., Anna Dreber, Eskil Forsell, Teck-Hua Ho, Jürgen Huber, Magnus Johannesson, Michael Kirchler, et al. 2016. “Evaluating Replicability of Laboratory Experiments in Economics.” *Science* 351 (6280): 1433–6. <https://doi.org/10.1126/science.aaf0918>.
- Camerer, Colin F., Anna Dreber, Felix Holzmeister, Teck-Hua Ho, Jürgen Huber, Magnus Johannesson, Michael Kirchler, et al. 2018. “Evaluating the Replicability of Social Science Experiments in Nature and Science Between 2010 and 2015.” *Nature Human Behaviour* 2 (9): 637.
- Collaboration, Open Science, and others. 2015. “Estimating the Reproducibility of Psychological Science.” *Science* 349 (6251): aac4716.
- Dirks, P. H., E. M. Roberts, H. Hilbert-Wolf, J. D. Kramers, J. Hawks, A. Dosseto, M. Duval, et al. 2017. “The Age of Homo Naledi and Associated Sediments in the Rising Star Cave, South Africa.” Journal Article. *Elife* 6. <https://doi.org/10.7554/eLife.24231>.
- Edwards, RL, CD Gallup, and H Cheng. 2003. “Uranium-Series Dating of Marine and Lacustrine Carbonates.” Journal Article. *Reviews in Mineralogy and Geochemistry* 52 (1): 363–405.
- Eggins, S. M., L. P. J. Kinsley, and J. M. G. Shelley. 1998. “Deposition and Element Fractionation Processes During Atmospheric Pressure Laser Sampling for Analysis by Icp-Ms.” Journal Article. *Applied Surface Science* 127–129 (0): 278–86. [https://doi.org/http://dx.doi.org/10.1016/S0169-4332\(97\)00643-0](https://doi.org/http://dx.doi.org/10.1016/S0169-4332(97)00643-0).
- Eggins, Stephen M., Rainer Grün, Malcolm T. McCulloch, Alistair W. G. Pike, John Chappell, Les Kinsley, Graham Mortimer, et al. 2005. “In Situ U-Series Dating by Laser-Ablation Multi-Collector Icpms: New Prospects for Quaternary Geochronology.” Journal Article. *Quaternary Science Reviews* 24 (23-24): 2523–38. <https://doi.org/10.1016/j.quascirev.2005.07.006>.
- Freedman, Leonard P, Iain M Cockburn, and Timothy S Simcoe. 2015. “The Economics of Reproducibility in Preclinical Research.” *PLoS Biology* 13 (6): e1002165.
- Gil, Yolanda, Cédric H. David, Ibrahim Demir, Bakinam T. Essawy, Robinson W. Fulweiler, Jonathan L. Goodall, Leif Karlstrom, et al. 2016. “Toward the Geoscience Paper of the Future: Best Practices for Documenting and Sharing Research from Data to Software to Provenance.” *Earth and Space Science* 3 (10): 388–415. <https://doi.org/10.1002/2015EA000136>.
- Grün, Rainer, Stephen Eggins, Leslie Kinsley, Hannah Moseley, and Malcolm Sambridge. 2014. “Laser Ablation U-Series Analysis of Fossil Bones and Teeth.” Journal Article. *Palaeogeography, Palaeoclimatology, Palaeoecology* 416: 150–67. <https://doi.org/http://dx.doi.org/10.1016/j.palaeo.2014.07.023>.
- Hutton, Christopher, Thorsten Wagener, Jim Freer, Dawei Han, Chris Duffy, and Berit Arheimer. 2016. “Most Computational Hydrology Is Not Reproducible, so Is It Really Science?” *Water Resources Research* 52 (10): 7548–55. <https://doi.org/10.1002/2016WR019285>.

- Institute, Global Biological Standards. 2013. “The Case for Standards in Life Science Research: Seizing Opportunities at a Time of Critical Need.”
- Ioannidis, John PA. 2005. “Why Most Published Research Findings Are False.” *PLoS Medicine* 2 (8): e124.
- Kattge, Jens, Sandra Díaz, and Christian Wirth. 2014. “Of Carrots and Sticks.” *Nature Geoscience* 7 (October): 778.
- Ludwig, KR. 2003. “Mathematical–Statistical Treatment of Data and Errors for $^{230}\text{Th}/\text{U}$ Geochronology.” Journal Article. *Reviews in Mineralogy and Geochemistry* 52 (1): 631–56.
- Ludwig, K. R. 2003. *User’s Manual for Isoplot 3.00*. Book. Berkeley, CA, USA: Berkeley Geochronology Center.
- Ludwig, K. R., and J. B. Paces. 2002. “Uranium-Series Dating of Pedogenic Silica and Carbonate, Crater Flat, Nevada.” Journal Article. *Geochimica et Cosmochimica Acta* 66 (3): 487–506. [https://doi.org/Doi:10.1016/S0016-7037\(01\)00786-4](https://doi.org/Doi:10.1016/S0016-7037(01)00786-4).
- Ludwig, K. R., and D. M. Titterton. 1994. “Calculation of $^{230}\text{Th}/\text{U}$ Isochrons, Ages, and Errors.” Journal Article. *Geochimica et Cosmochimica Acta* 58 (22): 5031–42. [https://doi.org/http://dx.doi.org/10.1016/0016-7037\(94\)90229-1](https://doi.org/http://dx.doi.org/10.1016/0016-7037(94)90229-1).
- Luo, Xiaozhong, Mark Rehkämper, Der-Chuen Lee, and Alex N. Halliday. 1997. “High Precision $^{230}\text{Th}/^{232}\text{Th}$ and $^{234}\text{U}/^{238}\text{U}$ Measurements Using Energy-Filtered Icp Magnetic Sector Multiple Collector Mass Spectrometry.” Journal Article. *International Journal of Mass Spectrometry and Ion Processes* 171 (1–3): 105–17. [https://doi.org/http://dx.doi.org/10.1016/S0168-1176\(97\)00136-5](https://doi.org/http://dx.doi.org/10.1016/S0168-1176(97)00136-5).
- Ma, Xiaogang. 2018. “Data Science for Geoscience: Leveraging Mathematical Geosciences with Semantics and Open Data.” In *Handbook of Mathematical Geosciences*, 687–702. Springer.
- Marwick, Ben. 2016. “Computational Reproducibility in Archaeological Research: Basic Principles and a Case Study of Their Implementation.” *Journal of Archaeological Method and Theory*, 1–27. <https://doi.org/10.1007/s10816-015-9272-9>.
- Medical Sciences, Academy of. 2015. “Reproducibility and Reliability of Biomedical Research: Improving Research Practice.” In *Symposium Report*.
- Miguel, Edward, Colin Camerer, Katherine Casey, Joshua Cohen, Kevin M Esterling, Alan Gerber, Rachel Glennerster, et al. 2014. “Promoting Transparency in Social Science Research.” *Science* 343 (6166): 30–31.
- Nosek, Brian A, George Alter, George C Banks, Denny Borsboom, Sara D Bowman, Steven J Breckler, Stuart Buck, et al. 2015. “Promoting an Open Research Culture.” *Science* 348 (6242): 1422–5.
- Pan, Tsun-You, Colin V. Murray-Wallace, Anthony Dosseto, and Robert P. Bourman. 2018. “The Last Interglacial (Mis 5e) Sea Level Highstand from a Tectonically Stable Far-Field Setting, Yorke Peninsula, Southern Australia.” Journal Article. *Marine Geology* 398: 126–36. <https://doi.org/10.1016/j.margeo.2018.01.012>.

- Pebesma, Edzer, Daniel Nüst, and Roger Bivand. 2012. “The R Software Environment in Reproducible Geoscientific Research.” *Eos, Transactions American Geophysical Union* 93 (16): 163–63. <https://doi.org/10.1029/2012EO160003>.
- Richards, David A, and Jeffrey A Dorale. 2003. “Uranium-Series Chronology and Environmental Applications of Speleothems.” Journal Article. *Reviews in Mineralogy and Geochemistry* 52 (1): 407–60.
- Sambridge, M., R. Grün, and S. Eggins. 2012. “U-Series Dating of Bone in an Open System: The Diffusion-Adsorption-Decay Model.” Journal Article. *Quaternary Geochronology*. <http://www.scopus.com/inward/record.url?eid=2-s2.0-84857958926&partnerID=40&md5=01e7f1b7d3554da26b247125425ff496>.
- Sutikna, Thomas, Matthew W. Tocheri, Michael J. Morwood, E. Wahyu Saptomo, Jatmiko, Rokus Due Awe, Sri Wasisto, et al. 2016. “Revised Stratigraphy and Chronology for Homo Floresiensis at Liang Bua in Indonesia.” Journal Article. *Nature* 532 (7599): 366–69. <https://doi.org/10.1038/nature17179>.
- Wickham, Hadley, and Jennifer Bryan. 2018. *Readxl: Read Excel Files*. <https://CRAN.R-project.org/package=readxl>.

Colophon

This report was generated on 2020-10-28 23:55:37 using the following computational environment and dependencies:

```
# which R packages and versions?
devtools::session_info()
```

```
## - Session info -----
## setting      value
## version      R version 4.0.2 (2020-06-22)
## os           macOS Catalina 10.15.6
## system       x86_64, darwin17.0
## ui           X11
## language     (EN)
## collate      en_US.UTF-8
## ctype        en_US.UTF-8
## tz           America/Los_Angeles
## date         2020-10-28
##
## - Packages -----
## package      * version date      lib source
## assertthat    0.2.1   2019-03-21 [2] CRAN (R 4.0.0)
## backports     1.1.10  2020-09-15 [2] CRAN (R 4.0.2)
## bookdown      0.21    2020-10-13 [2] CRAN (R 4.0.2)
## callr         3.5.1   2020-10-13 [2] CRAN (R 4.0.2)
## cli           2.1.0   2020-10-12 [2] CRAN (R 4.0.2)
## colorspace    1.4-1   2019-03-18 [2] CRAN (R 4.0.0)
## cowplot       1.1.0   2020-09-08 [2] CRAN (R 4.0.2)
## crayon        1.3.4   2017-09-16 [2] CRAN (R 4.0.0)
## desc          1.2.0   2018-05-01 [2] CRAN (R 4.0.0)
## deSolve       1.28    2020-03-08 [2] CRAN (R 4.0.0)
## devtools      2.3.2   2020-09-18 [2] CRAN (R 4.0.2)
## digest        0.6.27  2020-10-24 [2] CRAN (R 4.0.2)
## dplyr          * 1.0.2   2020-08-18 [2] CRAN (R 4.0.2)
## ellipsis      0.3.1   2020-05-15 [2] CRAN (R 4.0.0)
## evaluate      0.14    2019-05-28 [2] CRAN (R 4.0.0)
## fansi         0.4.1   2020-01-08 [2] CRAN (R 4.0.0)
## farver        2.0.3   2020-01-16 [2] CRAN (R 4.0.0)
## fs            1.5.0   2020-07-31 [2] CRAN (R 4.0.2)
## generics      0.0.2   2018-11-29 [2] CRAN (R 4.0.0)
## ggplot2       * 3.3.2   2020-06-19 [2] CRAN (R 4.0.0)
## glue          1.4.2   2020-08-27 [2] CRAN (R 4.0.2)
## gtable        0.3.0   2019-03-25 [2] CRAN (R 4.0.0)
## htmltools     0.5.0   2020-06-16 [2] CRAN (R 4.0.0)
## knitr         * 1.30    2020-09-22 [2] CRAN (R 4.0.2)
## labeling      0.4.2   2020-10-20 [2] CRAN (R 4.0.2)
```

```
## lifecycle      0.2.0    2020-03-06 [2] CRAN (R 4.0.0)
## magrittr       1.5      2014-11-22 [2] CRAN (R 4.0.0)
## memoise        1.1.0    2017-04-21 [2] CRAN (R 4.0.0)
## munsell         0.5.0    2018-06-12 [2] CRAN (R 4.0.0)
## pillar         1.4.6    2020-07-10 [2] CRAN (R 4.0.0)
## pkgbuild        1.1.0    2020-07-13 [2] CRAN (R 4.0.0)
## pkgconfig       2.0.3    2019-09-22 [2] CRAN (R 4.0.0)
## pkgload         1.1.0    2020-05-29 [2] CRAN (R 4.0.0)
## prettyunits     1.1.1    2020-01-24 [2] CRAN (R 4.0.0)
## processx        3.4.4    2020-09-03 [2] CRAN (R 4.0.2)
## ps              1.4.0    2020-10-07 [2] CRAN (R 4.0.2)
## purrr           0.3.4    2020-04-17 [2] CRAN (R 4.0.0)
## R6              2.5.0    2020-10-28 [2] CRAN (R 4.0.2)
## remotes         2.2.0    2020-07-21 [2] CRAN (R 4.0.2)
## rlang           0.4.8    2020-10-08 [2] CRAN (R 4.0.2)
## rmarkdown       2.4.6    2020-10-19 [2] Github (rstudio/rmarkdown@7239cea)
## rprojroot       1.3-2    2018-01-03 [2] CRAN (R 4.0.0)
## rticles         0.16     2020-09-22 [2] CRAN (R 4.0.2)
## scales          1.1.1    2020-05-11 [2] CRAN (R 4.0.0)
## sessioninfo     1.1.1    2018-11-05 [2] CRAN (R 4.0.0)
## stringi         1.5.3    2020-09-09 [2] CRAN (R 4.0.2)
## stringr         1.4.0    2019-02-10 [2] CRAN (R 4.0.0)
## testthat        2.3.2    2020-03-02 [2] CRAN (R 4.0.0)
## tibble          3.0.4    2020-10-12 [2] CRAN (R 4.0.2)
## tidyselect      1.1.0    2020-05-11 [2] CRAN (R 4.0.0)
## usethis         1.6.3    2020-09-17 [2] CRAN (R 4.0.2)
## UThwigl         * 0.1.0    2020-10-29 [1] local
## vctrs           0.3.4    2020-08-29 [2] CRAN (R 4.0.2)
## withr           2.3.0    2020-09-22 [2] CRAN (R 4.0.2)
## xfun            0.18     2020-09-29 [2] CRAN (R 4.0.2)
## xtable          * 1.8-4    2019-04-21 [2] CRAN (R 4.0.2)
## yaml            2.2.1    2020-02-01 [2] CRAN (R 4.0.0)
##
## [1] /private/var/folders/mz/6nn330m17_37ck5hhz2p24100000gn/T/Rtmpx0h6q0/temp_libpathfd17
## [2] /Library/Frameworks/R.framework/Versions/4.0/Resources/library
```

The current Git commit details are:

```
# git2r::repository(here::here())
```