

iDADwigl - an R package for open-system uranium-thorium dating

Anthony Dosseto^{*,a}, Ben Marwick^b

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

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

Abstract

This is the abstract.

It consists of two paragraphs.

*Corresponding Author

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

1 Introduction

2 Open-system uranium-thorium (U-Th) dating of teeth and bones, while chal-
3 lenging, has revolutionised our ability to provide reliable chronology for humans
4 and fauna (Eggins et al. 2005; Grün et al. 2014; Sambridge, Grün, and Eggins
5 2012). Thus, this approach has significantly improved our understanding of hu-
6 man evolution (e.g. Dirks et al. 2017; Sutikna et al. 2016). Uranium-thorium
7 dating is based on the premise that a material takes up U but no Th, so all the
8 ^{230}Th in the sample comes from decay of ^{238}U . If detrital Th is included to the
9 sample, a correction must be included to account for the fraction of ^{230}Th which
10 is detrital and not derived from ^{238}U decay. Another requirement is that there
11 is no gain or loss of ^{230}Th , ^{234}U or ^{238}U after formation of the material. While it
12 is often the case for many geological samples such as corals or speleothems, this
13 requirement is rarely met for teeth and bone (although enamel can sometimes be
14 quite impervious to isotope gain or loss). Thus, for teeth and bone, U-Th dating
15 requires to take into account open system behaviour. The diffusion-adsorption-
16 decay (DAD) model developed by Sambridge et al. (2012) was instrumental to
17 implement successfully open-system U-Th dating. It allows for advective and
18 diffusive transport of uranium and thorium isotopes, while include synchronous
19 radioactive decay. The software implementation was written in Fortran and is
20 available as a Java GUI (<http://www.earth.org.au/codes/iDaD/>). In this arti-
21 cle, we propose a R package which implements the model of Sambridge et al.
22 (2012).

23 The motivation for providing this model as an R package is to increase
24 the transparency, reproducibility, and flexibility of the analytical workflow for
25 computing U-Th ages. Currently it is difficult to include the Java GUI in a
26 fully scripted data analysis so the method for computing the DAD model is not
27 highly transparent. This can obscure steps where key decisions are made that
28 are important for others to see to verify the reliability of the analysis. Enabling
29 a scripted workflow for computational analysis of geoscience data is important
30 for improving the reproducibility of results. Reproducibility refers the ability to
31 recreate the results or retest the hypotheses leading to a scientific claim, either
32 by rerunning the same code used by the original authors, or by writing new
33 code. High rates of irreproducibility of research results have been estimated
34 in several fields and disciplines (Medical Sciences 2015; Freedman, Cockburn,
35 and Simcoe 2015; Institute 2013; Ioannidis 2005; Collaboration and others 2015;
36 Camerer et al. 2018, 2016). Consequently, the transparency, openness, and
37 reproducibility of results and methods are receiving increased attention, and
38 the norms of research in many fields are changing (Nosek et al. 2015; Miguel et
39 al. 2014; Marwick 2016).

40 There is strong interest in open, transparent, and reusable research in the
41 geoscience community (Gil et al. 2016) and substantial progress toward open
42 data has been made in the geosciences with the widespread use of data services
43 of NASA, USGS, NOAA and community-built data portals such as OneGeol-
44 ogy, EarthChem, RRUFF, PANGAEA, PaleoBioDB, and others (Kattge, Díaz,
45 and Wirth 2014; Ma 2018). However, the use of open source software such

46 as R (Pebesma, Nüst, and Bivand 2012), and sharing of scripted data analy-
47 sis workflows with research publications is not yet widespread (Hutton et al.
48 2016). With this R package our goal is to make scripted and reproducible data
49 analysis easy for open-system uranium-thorium dating. This will improve the
50 transparency of geochronology research, and provide a more credible and robust
51 foundation for scientific advancement (Hutton et al. 2016).

52 To enable re-use of our materials and improve reproducibility and trans-
53 parency, all the results and visualisations in this paper can be reproduced using
54 the RMarkdown vignette document included with the iDADwogl package. We
55 have archived these files at <http://doi.org/XXX/XXX> to ensure long-term ac-
56 cessibility. Our code is released under the MIT licence, our data as CC-0, and
57 our figures as CC-BY, to enable maximum re-use (for more details, see Marwick
58 2016).

59 Methods

60 Data required for the DAD model are ($^{230}\text{Th}/^{238}\text{U}$) and ($^{234}\text{U}/^{238}\text{U}$) activity
61 ratios collected along a transect perpendicular to the surface of the tooth or
62 bone (brackets denote activity ratios throughout this article). Sampling for
63 analysis can be done by micro-drilling or laser ablation. If the former, aliquots
64 are then dissolved, followed by separation of U and Th using ion exchange
65 chromatography. This is more time consuming (at least one week of work) than
66 laser ablation, where the material sampled by the laser is directly sent to the
67 mass spectrometer.

68 While laser ablation also offers a better spatial resolution than micro-drilling,
69 the precision of the data is inferior because of the much smaller amount of
70 material sampled. Uranium and thorium isotope ratios are then analysed by
71 multi-collector inductively-coupled plasma mass spectrometry. A plasma ionise
72 all U and Th atoms, their isotopes are separated through a magnetic field and
73 each collected in a different collector. If using laser ablation, it is best to have
74 two ion counters so ^{230}Th and ^{234}U can be collected simultaneously.

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

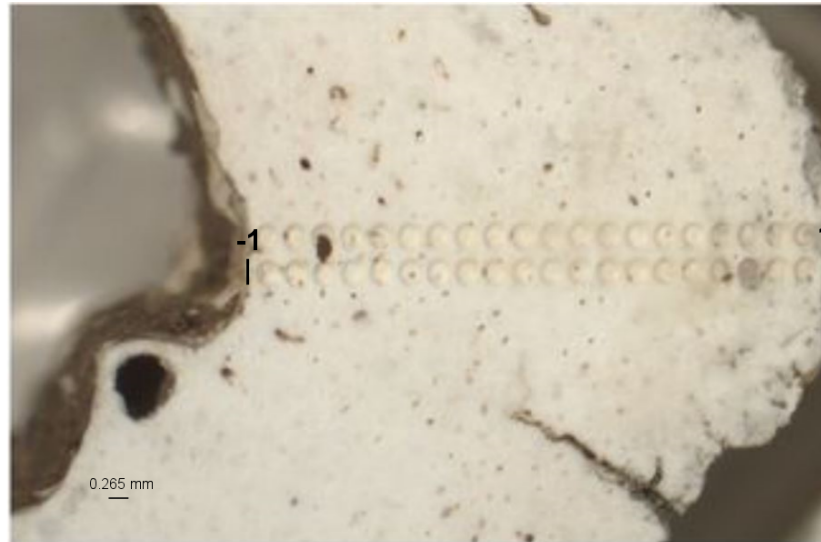


Figure 1: Modern human femur (132A/LB/27D/03) from Liang Bua, Flores, Indonesia. Two analysis transects can be seen. For a given transect, the outer and inner surface of the bone are given 1 and -1 reference coordinates, and the position of each analysis is calculated accordingly. Modified from Sutikna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

79 Installing and attaching the package

80 To run the model, start R and install the package from GitHub. There are
 81 many ways to do this, one simple method is shown in the line below. This only
 82 needs to be done once per computer.

```
source("https://install-github.me/tonydoss/iDADwigl")
```

83 For routine data analysis, R scripts need to contain this line to attach the
 84 package to the current working environment. This line needs to be run at the
 85 start of each analysis:

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

86 Input data format

87 The key function of our package, `iDADwig1()` requires a data frame (a form
88 of table in R) with the following column names:

- 89 • `iDAD.position`
- 90 • `U234_U238_CORR`
- 91 • `U234_U238_CORR_Int2SE`
- 92 • `iDAD.position.1`
- 93 • `Th230_U238_CORR`
- 94 • `Th230_U238_CORR_Int2SE`
- 95 • `U_ppm`
- 96 • `U_ppm_Int2SE`

97 This data frame can be created by importing an Excel or CSV file into the R
98 environment using a generic function such as `read.csv` or `read_excel` from the
99 `readxl` package (Wickham and Bryan 2018). To help with preparing data for
100 input into our function, we have included two examples of input files. The code
101 chunk below shows how to access one of the two example CSV files included in
102 the package, and how to read it into the R environment.

```
# get the path the one of the CSV files included in the package
path_to_included_example_csv_file <-
  system.file("extdata",
              "input/Hobbit_MH2T_for_iDAD.csv",
              package = "iDADwig1",
              mustWork = TRUE)

# read in the example CSV file included in the package
Hobbit_MH2T_for_iDAD <-
  read.csv(path_to_included_example_csv_file)
```

Table 1 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	0.00	12.3	0.615
-0.857	1.273	0.004	-0.857	0.073	0.00	12.7	0.635
-0.758	1.265	0.004	-0.758	0.076	0.00	12.5	0.625
-0.659	1.267	0.005	-0.659	0.077	0.00	14.2	0.710
-0.560	1.269	0.003	-0.560	0.072	0.00	19.8	0.990
-0.461	1.266	0.003	-0.461	0.077	0.00	18.0	0.900
-0.361	1.267	0.003	-0.361	0.082	0.00	20.0	1.000
-0.262	1.276	0.002	-0.262	0.079	0.00	27.2	1.360
-0.163	1.266	0.002	-0.163	0.075	0.00	26.7	1.335
-0.064	1.277	0.002	-0.064	0.073	0.00	0.3	0.015
0.035	1.271	0.002	0.035	0.078	0.00	33.9	1.695
0.134	1.264	0.002	0.134	0.067	0.00	37.7	1.885
0.233	1.266	0.003	0.233	0.071	0.00	30.7	1.535
0.332	1.265	0.002	0.332	0.077	0.00	25.2	1.260
0.431	1.266	0.003	0.431	0.083	0.00	28.9	1.445
0.530	1.268	0.003	0.530	0.086	0.00	29.0	1.450
0.629	1.264	0.003	0.629	0.082	0.00	27.5	1.375
0.728	1.263	0.002	0.728	0.070	0.00	30.1	1.505
0.827	1.266	0.005	0.827	0.095	0.00	19.6	0.980
0.926	1.263	0.003	0.926	0.096	0.00	14.8	0.740

Table 1: Data contained in the example CSV file `Hobbit_MH2T_for_iDAD.csv` included in the package

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 `iDADwig1()` 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. The order of the columns in the data frame is not important.

113 The `iDAD.position` column corresponds to the coordinates of the ($^{234}\text{U}/^{238}\text{U}$)
 114 analyses, which as indicated above take values between -1 and 1 (Figure 1). The
 115 second `iDAD.position.1` column is used if the coordinates of the ($^{230}\text{Th}/^{238}\text{U}$)
 116 analyses are different from those of the ($^{234}\text{U}/^{238}\text{U}$) analyses.
 117 Columns `U234_U238_CORR` and `U234_U238_CORR_Int2SE` are the ($^{234}\text{U}/^{238}\text{U}$)
 118 activity ratios and their 2σ errors. Columns `Th230_U238_CORR` and `Th230_U238_CORR_Int2SE`
 119 are the ($^{230}\text{Th}/^{238}\text{U}$) activity ratios and their 2σ errors.
 120 Columns `U_ppm` and `U_ppm_Int2SE` and calculated uranium concentrations
 121 (in ppm) and their 2σ errors. Uranium concentrations are not necessary for the
 122 model and only used for display of the U concentration profile in a figure.

123 **Details of the input parameters**

124 Our key function, `iDADwigl()` has several arguments that need to be set
 125 before we can get meaningful results.

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

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

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

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

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

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

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

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

155 How to run the model

156 To run the function, attach the package and then run `iDADwigl()`, specifying
157 the input data frame and the input parameters as described above. The code
158 block below shows a quick example that will execute in less than five seconds
159 on a typical 2.3 GHz Intel Core i5 laptop:

```
output <- iDADwigl(Hobbit_MH2T_for_iDAD,  
  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)
```

160 When run on the R console, this function will print a confirmation that the
161 input data frame has the required columns, and print the resulting age value
162 with an error reported as the 67% and 33% quantiles, for instance:

```
163 All required columns are present in the input data  
164 [1] "Age: 7 +0.6/-0.7 ka"
```

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

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

178 In a typical analysis we will explore the model fit by first running the model
179 with a single iteration `nbit` and a small value for `fsum_target`, and then chang-
180 ing the range of allowed values for the ($^{234}\text{U}/^{238}\text{U}$) ratio at the surface and the
181 age of the sample. Once we obtain a satisfying fit (by visual inspection of the
182 produced figures), we would increase `nbit` to a higher value (e.g. 1000) and run
183 the model one last time. See below for an example of analysis.

184 *Inspecting the model's output*

185 `T_final`, `K_final` and `U48_0_final` are included in the model's output,
 186 along with their uncertainties. The function also includes a one-row data frame
 187 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
6.96	0.64	0.62	1.2699	0.0001	0.0049

Table 2: Summary table of the computed age and error values

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

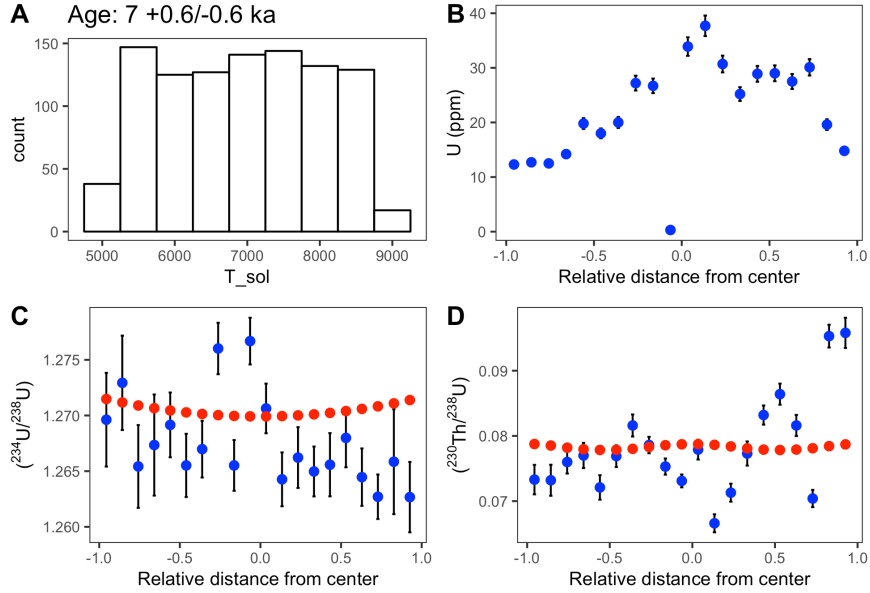


Figure 2: Example of the visualisations produced by the `iDADwig1()` function, using the demonstration run described above. A: Histogram of the solution ages, B: Uranium concentration profile for transect 2 of modern human femur 132A/LB/27D/03. C: Calculated (red) and observed (blue) $^{234}\text{U}/^{238}\text{U}$ 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.

Visualising the model's output

`iDADwig1()` returns several figures useful for visualisation of the model results along with the data:

1. a histogram of the solution ages (Figure 2 A)
2. the U concentrations in the sample as a function of the relative distance from the center (Figure 2 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 2 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 2 D).

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

Table 3: Example of output table including the input data described above, and two new columns

Case study of two ages from Sutikna et al. 2016

The package includes two sample data sets derived from Sutikna et al. (2016) : “Hobbit_MH2T_for_iDAD.csv” is data from transect 2 for modern human femur 132A/LB/27D/03 (shown above in Table 1). “Hobbit_11T_for_iDAD.csv” is data from transect 1 for *Homo floresiensis* ulna LB1/52 (Table 4). For the latter, six analyses were removed from the set as in Sutikna 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	0.01	32.0	1.600
0.165	1.370	0.002	0.165	0.733	0.01	41.1	2.055
0.319	1.364	0.002	0.319	0.672	0.01	35.8	1.790
0.472	1.362	0.003	0.472	0.636	0.01	27.6	1.380
0.626	1.365	0.003	0.626	0.641	0.01	31.0	1.550
0.780	1.374	0.003	0.780	0.712	0.01	27.9	1.395

Table 4: Data contained in the example CSV file Hobbit_11T_for_iDAD.csv included in the package

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

For transect 2 of 132A/LB/27D/03, Sutikna et al. (2016) reported an age of 7.4 ± 0.5 ka (thousand years before 2014). With iDADwgl, we first run the model with `nbit = 1`, `fsum_target = 0.05`, `U48_0_min` and `U48_0_max` = 1.25 and 1.3, respectively, `l = 5.35` cm, `U_0 = 25` ppm, `K_min` and `K_max` = 10^{-13} and 10^{-11} cm²/s, respectively, `T_min` and `T_max` = 10^3 and 500×10^3 yr, respectively. `U48_0_min` and `U48_0_max` are determined by considering the measured ($^{234}\text{U}/^{238}\text{U}$) values near the surfaces of the sample. `T_min` and `T_max` values were chosen such that no a priori knowledge of the age biases the results.

With this first run, we obtain an age of 8 ka. There is no calculated error on the age since there is only one iteration. As we can see, the calculated ($^{234}\text{U}/^{238}\text{U}$) and ($^{230}\text{Th}/^{238}\text{U}$) ratios are higher than observed values (Figure 4). For the ($^{234}\text{U}/^{238}\text{U}$), it makes sense to thus use a narrower range for `U48_0_min` and `U48_0_max`. Higher calculated ($^{230}\text{Th}/^{238}\text{U}$) ratios compared to observed values suggests that the calculated age is too old (since this ratio increases with age). Thus, we should consider a lower value for `T_max`.

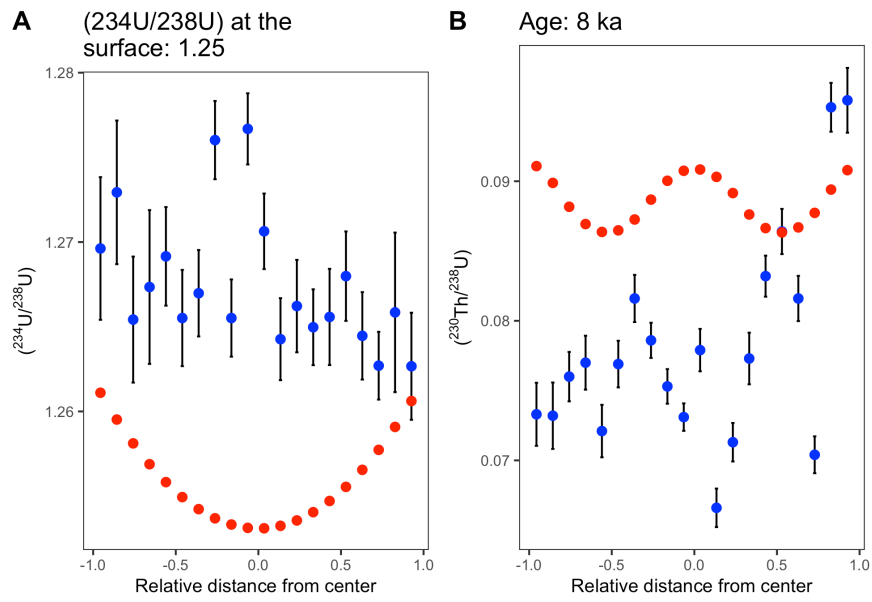


Figure 3: Results from the model's first run with the modern human femur. A: Calculated (red) and observed (blue) $(^{234}\text{U}/^{238}\text{U})$ activity ratios for transect 2 of modern human femur 132A/LB/27D/03. B: Calculated (red) and observed (blue) $(^{230}\text{Th}/^{238}\text{U})$ activity ratios for transect 2 of modern human femur 132A/LB/27D/03.

224 The model is thus run a second time, increasing the number of iterations to
225 1000, and changing `U48_0_min` and `U48_0_max` to 1.265 and 1.270, respectively,
226 and `T_max` to 10^3 yr. Since the first run suggests a Holocene age for the sample,
227 the measured ($^{234}\text{U}/^{238}\text{U}$) at the surfaces must be similar to the calculated
228 values, thus the chosen values for the range above.

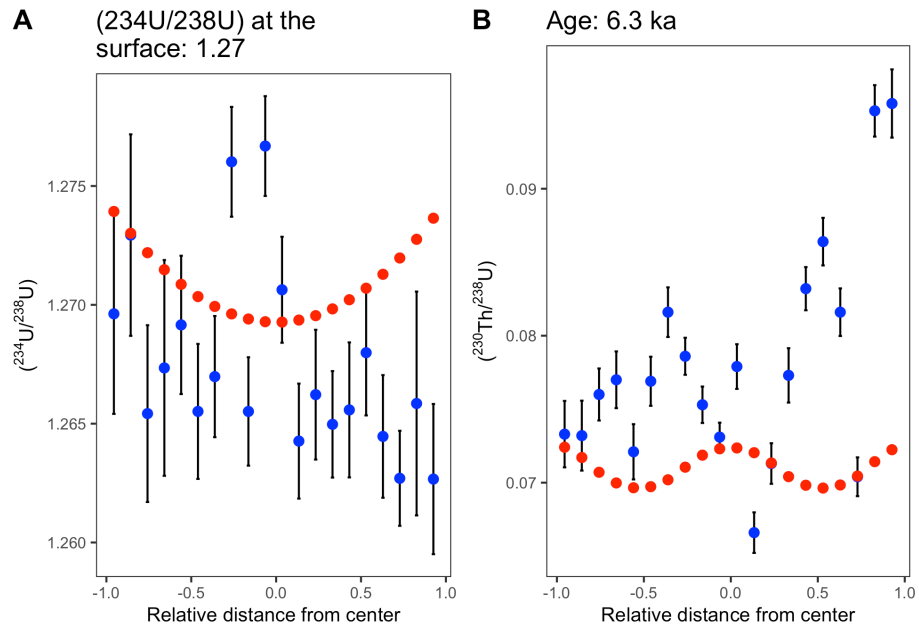


Figure 4: Results from the model's second run with the modern human femur. A: Calculated (red) and observed (blue) $(^{234}\text{U}/^{238}\text{U})$ activity ratios for transect 2 of modern human femur 132A/LB/27D/03. B: Calculated (red) and observed (blue) $(^{230}\text{Th}/^{238}\text{U})$ activity ratios for transect 2 of modern human femur 132A/LB/27D/03.

229 U48_0_min, U48_0_min, T_min and T_max can be further adjusted. `fsum_target`
230 can also be decreased to 0.01 in order to get a better fit and error, but it is at
231 the expense of computing time. Once a satisfying fit is obtained (assessed by
232 inspecting the figures produced), the number of iterations `nbit` can be increased
233 to 1000 (or higher). Following this method, we obtain an age of $6.3 \pm 1.3/-1.1$
234 ka (Figure 4).

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

236 For transect 1 of LB1/52, Sutikna et al. (2016) reported an age of 79.0
237 ± 3.7 ka. With iDADwigl, using data in the file `Hobbit_1-1T_for_iDAD.csv`
238 provided in the package, and following the same method as above, we obtain
239 an age of $75.5 \pm 1/-1$ ka (Figure 5).

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

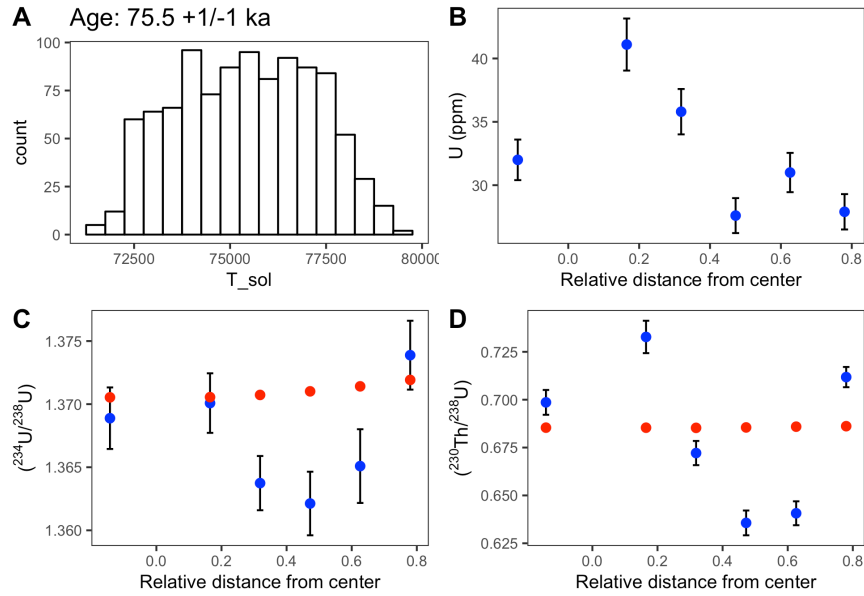


Figure 5: Results from running the model with *Homo floresiensis* ulna LB1/52 data from Sutikna et al. (2016). A: Histogram of the solution ages, B: Uranium concentration profile for transect 1 of *Homo floresiensis* ulna LB1/52. C: Calculated (red) and observed (blue) $(^{234}U/^{238}U)$ activity ratios for transect 1 of *Homo floresiensis* ulna LB1/52. D: Calculated (red) and observed (blue) $(^{230}Th/^{238}U)$ activity ratios for transect 1 of *Homo floresiensis* ulna LB1/52.

Conclusions

In this paper we have described `iDADwig1`, 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>.
- 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.
- 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.
- 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>.
- 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 2018-12-25 14:50:09 using the following computational environment and dependencies:

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

```
## - Session info -----  
## setting value  
## version R version 3.5.1 (2018-07-02)  
## os      macOS 10.14.2  
## system x86_64, darwin15.6.0  
## ui      X11  
## language (EN)  
## collate en_US.UTF-8  
## ctype   en_US.UTF-8  
## tz      America/Los_Angeles  
## date    2018-12-25  
##  
## - Packages -----  
## package * version      date      lib  
## assertthat 0.2.0      2017-04-11 [1]  
## backports  1.1.3      2018-12-14 [1]  
## bookdown    0.9        2018-12-21 [1]  
## callr       3.1.1      2018-12-21 [1]  
## cli         1.0.1      2018-09-25 [1]  
## codetools   0.2-15     2016-10-05 [1]  
## colorspace  1.3-2      2016-12-14 [1]  
## cowplot     * 0.9.3      2018-07-15 [1]  
## crayon      1.3.4      2018-12-18 [1]  
## desc        1.2.0      2018-05-01 [1]  
## devtools    2.0.1      2018-10-26 [1]  
## digest      0.6.18     2018-10-10 [1]  
## dplyr        * 0.7.99.9000 2018-12-25 [1]  
## evaluate    0.12       2018-10-09 [1]  
## fs          1.2.6      2018-08-23 [1]  
## ggplot2     * 3.1.0.9000 2018-12-25 [1]  
## glue        1.3.0      2018-10-31 [1]  
## gtable      0.2.0      2016-02-26 [1]  
## here        0.1        2017-05-28 [1]  
## htmltools   0.3.6      2017-04-28 [1]  
## iDADwgl     * 0.1.0      2018-12-25 [1]  
## knitr        * 1.21       2018-12-10 [1]  
## labeling    0.3        2014-08-23 [1]  
## lazyeval    0.2.1      2017-10-29 [1]  
## magrittr    1.5        2014-11-22 [1]
```

```

## memoise      1.1.0      2017-04-21 [1]
## munsell      0.5.0      2018-06-12 [1]
## pillar      1.3.1.9000  2018-12-23 [1]
## pkgbuild     1.0.2      2018-10-16 [1]
## pkgconfig    2.0.2      2018-08-16 [1]
## pkgload      1.0.2      2018-10-29 [1]
## prettyunits  1.0.2      2015-07-13 [1]
## processx     3.2.1      2018-12-05 [1]
## ps           1.3.0      2018-12-21 [1]
## purrr        0.2.5      2018-05-29 [1]
## R6           2.3.0      2018-10-04 [1]
## Rcpp         1.0.0      2018-11-07 [1]
## remotes      2.0.2      2018-10-30 [1]
## rlang        0.3.0.1    2018-10-25 [1]
## rmarkdown    1.11      2018-12-08 [1]
## rprojroot    1.3-2      2018-01-03 [1]
## rticles      0.6        2018-10-09 [1]
## scales       1.0.0      2018-08-09 [1]
## sessioninfo  1.1.1      2018-11-05 [1]
## stringi      1.2.4      2018-07-20 [1]
## stringr      1.3.1      2018-05-10 [1]
## testthat     2.0.1      2018-10-13 [1]
## tibble       1.4.99.9006 2018-12-25 [1]
## tidyselect   0.2.5      2018-10-11 [1]
## usethis      1.4.0      2018-08-14 [1]
## withr        2.1.2      2018-03-15 [1]
## xfun         0.4        2018-10-23 [1]
## xtable       * 1.8-3     2018-08-29 [1]
## yaml         2.2.0      2018-07-25 [1]
## source
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.1)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## Github (gaborcsardi/crayon@74bee76)
## CRAN (R 3.5.0)
## CRAN (R 3.5.1)
## CRAN (R 3.5.0)
## Github (tidyverse/dplyr@bee3351)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## Github (tidyverse/ggplot2@7f13dfa)

```

```
## Github (tidyverse/glue@35c61e9)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## local
## CRAN (R 3.5.1)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## Github (r-lib/pillar@9cc3030)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## Github (tidyverse/tibble@f3b40c2)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
##
## [1] /Library/Frameworks/R.framework/Versions/3.5/Resources/library
```

The current Git commit details are:

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

```
## Local:      master /Users/bmarwick/Desktop/iDADwigl
```

```
## Remote:  master @ origin (https://github.com/benmarwick/iDADwigl.git)
## Head:      [298efc3] 2018-12-25: convert vignette into Elsevier article format, tidy table
```