

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

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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 a R package, named *iDADwigl* 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. Examples of application of the model are also provided, showing that it yields ages within error of previously published values.

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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 iDADwgl 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).

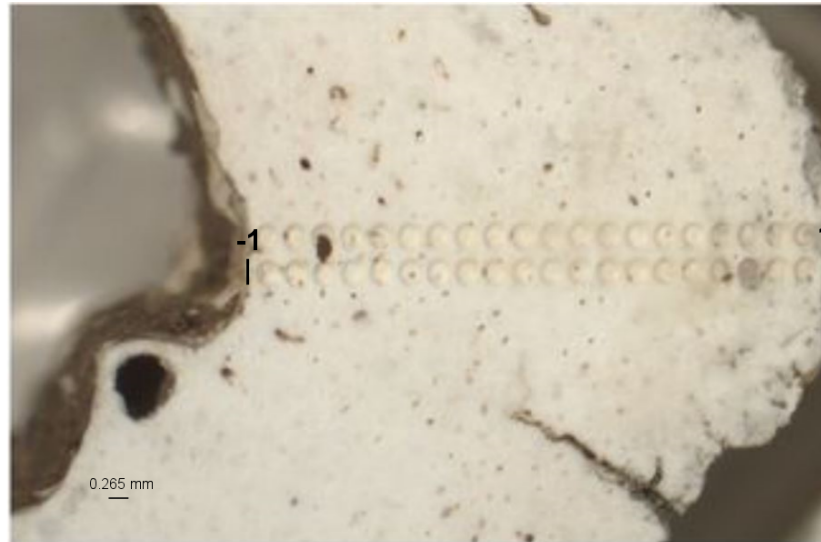


Figure 1: Modern human femur (132A/LB/27D/03) from Liang Bua, Flores, Indonesia. Two analysis transects can be seen. For a given transect, the outer and inner surface of the bone are given 1 and -1 reference coordinates, and the position of each analysis is calculated accordingly. Modified from Sutikna 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, `iDADwigl()` 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 To help with preparing data for input into our function, we have included
98 two examples of input files. Inspecting the included data sets will be helpful for
99 understanding how to prepare new data to prepare for use with this package.
100 After attaching the package, we can access the built-in datasets with the `data()`
101 function, like this:

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

102 This will make the built-in data available in the R environment to inspect
103 and explore how to use the `iDADwigl()` function.

104 To use new data with this package, we can import an Excel or CSV file into
105 the R environment using a generic function such as `read.csv` or `read_excel`
106 from the `readxl` package (Wickham and Bryan 2018). The code chunk below
107 shows how to read one of the CSV files included in the package into the R
108 environment. This is a good method to use if you supply your own CSV file
109 to use with `iDADwigl()`. In this case we assume that the working directory
110 contains a directory called `data` and our CSV file is in this `data` directory:

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

111 Table 1 shows the data contained in the `Hobbit_MH2T_for_iDAD.csv` file
112 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 1: Data contained in the example CSV file `Hobbit_MH2T_for_iDAD.csv` included in the package

113 The columns `iDAD.position`, `U234_U238_CORR`, `U234_U238_CORR_Int2SE`,
114 `Th230_U238_CORR` and `Th230_U238_CORR_Int2SE` must be present in the input
115 data frame with these exact names for the model to function. The `iDADwig1()`
116 function will check if the input data frame has these columns, and will stop
117 with an error message if it does not find these columns. The `names()` function
118 can be used to update column names of a data frame to ensure they match the
119 names that the model function requires. The order of the columns in the data
120 frame is not important.

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

131 **Details of the input parameters**

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

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

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

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

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

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

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

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

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

163 How to run the model

164 To run the function, attach the package and then run `iDADwigl()`, specifying
165 the input data frame and the input parameters as described above. The code
166 block below shows a quick example that will execute in less than five seconds
167 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)
```

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

```
171 All required columns are present in the input data  
172 [1] "Age: 7 +0.6/-0.7 ka"
```

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

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

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

192 *Inspecting the model's output*

193 T_final, K_final and U48_0_final are included in the model's output,
 194 along with their uncertainties. The function also includes a one-row data frame
 195 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
6.99	0.62	0.66	1.2662	0.0038	0.0012

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

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

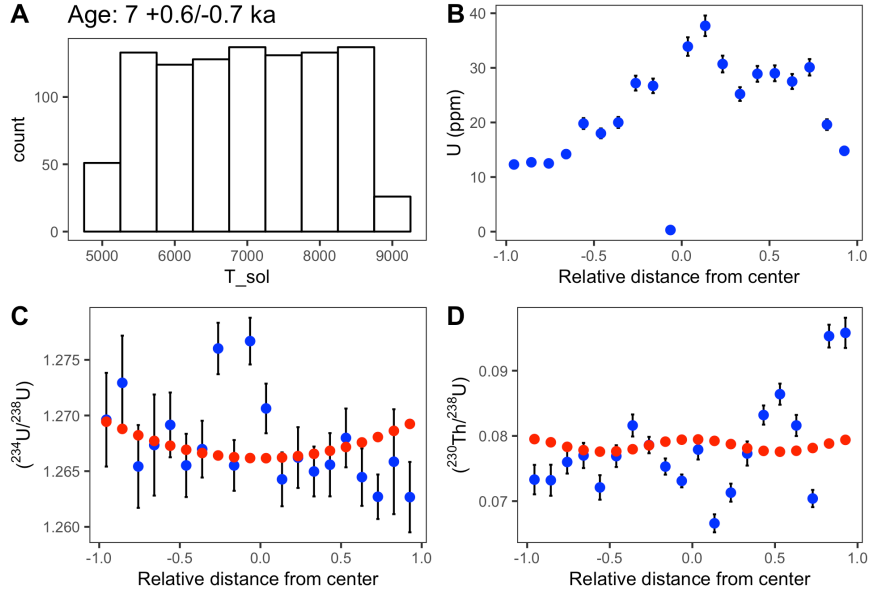


Figure 2: Example of the visualisations produced by the `iDADwig1()` function, using the demonstration run described above. A: Histogram of the solution ages, B: Uranium concentration profile for transect 2 of modern human femur 132A/LB/27D/03. C: Calculated (red) and observed (blue) $(^{234}\text{U}/^{238}\text{U})$ 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	1.269	0.080
-0.857	1.273	0.004	-0.857	0.073	0.002	12.7	0.6	1.269	0.079
-0.758	1.265	0.004	-0.758	0.076	0.002	12.5	0.6	1.268	0.078
-0.659	1.267	0.005	-0.659	0.077	0.002	14.2	0.7	1.268	0.078
-0.560	1.269	0.003	-0.560	0.072	0.002	19.8	1.0	1.267	0.078
-0.461	1.266	0.003	-0.461	0.077	0.002	18.0	0.9	1.267	0.078
-0.361	1.267	0.003	-0.361	0.082	0.002	20.0	1.0	1.267	0.078
-0.262	1.276	0.002	-0.262	0.079	0.001	27.2	1.4	1.266	0.079
-0.163	1.266	0.002	-0.163	0.075	0.001	26.7	1.3	1.266	0.079
-0.064	1.277	0.002	-0.064	0.073	0.001	0.3	0.0	1.266	0.079
0.035	1.271	0.002	0.035	0.078	0.002	33.9	1.7	1.266	0.079
0.134	1.264	0.002	0.134	0.067	0.001	37.7	1.9	1.266	0.079
0.233	1.266	0.003	0.233	0.071	0.001	30.7	1.5	1.266	0.079
0.332	1.265	0.002	0.332	0.077	0.002	25.2	1.3	1.267	0.078
0.431	1.266	0.003	0.431	0.083	0.001	28.9	1.4	1.267	0.078
0.530	1.268	0.003	0.530	0.086	0.002	29.0	1.4	1.267	0.078
0.629	1.264	0.003	0.629	0.082	0.002	27.5	1.4	1.268	0.078
0.728	1.263	0.002	0.728	0.070	0.001	30.1	1.5	1.268	0.078
0.827	1.266	0.005	0.827	0.095	0.002	19.6	1.0	1.269	0.079
0.926	1.263	0.003	0.926	0.096	0.002	14.8	0.7	1.269	0.079

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

209 **Case study of two ages from Sutikna et al. 2016**

210 The package includes two sample data sets derived from Sutikna et al.
 211 (2016) : “Hobbit_MH2T_for_iDAD.csv” is data from transect 2 for mod-
 212 ern human femur 132A/LB/27D/03 (shown above in Table 1). “Hobbit_1-
 213 1T_for_iDAD.csv” is data from transect 1 for *Homo floresiensis* ulna LB1/52
 214 (Table 4). For the latter, six analyses were removed from the set as in Sutikna
 215 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 4: Data contained in the example CSV file Hobbit_11T_for_iDAD.csv included in the package

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

217 For transect 2 of 132A/LB/27D/03, Sutikna et al. (2016) reported an age
 218 of 7.4 ± 0.5 ka (thousand years before 2014). With iDADwgl, we first run
 219 the model with `nbit = 1`, `fsum_target = 0.05`, `U48_0_min` and `U48_0_max`
 220 `= 1.25` and `1.3`, respectively, `l = 5.35` cm, `U_0 = 25` ppm, `K_min` and `K_max`
 221 `= 10-13` and `10-11` cm²/s, respectively, `T_min` and `T_max = 103` and `500x103`
 222 yr, respectively. `U48_0_min` and `U48_0_max` are determined by considering the
 223 measured (²³⁴U/²³⁸U) values near the surfaces of the sample. `T_min` and `T_max`
 224 values were chosen such that no a priori knowledge of the age biases the results.

225 With this first run, we obtain an age of 5.4 ka. There is no calculated error
 226 on the age since there is only one iteration. As we can see, the calculated
 227 (²³⁴U/²³⁸U) and (²³⁰Th/²³⁸U) ratios are higher than observed values (Figure 4).
 228 For the (²³⁴U/²³⁸U), it makes sense to thus use a narrower range for `U48_0_min`
 229 and `U48_0_max`. Higher calculated (²³⁰Th/²³⁸U) ratios compared to observed
 230 values suggests that the calculated age is too old (since this ratio increases with
 231 age). Thus, we should consider a lower value for `T_max`.

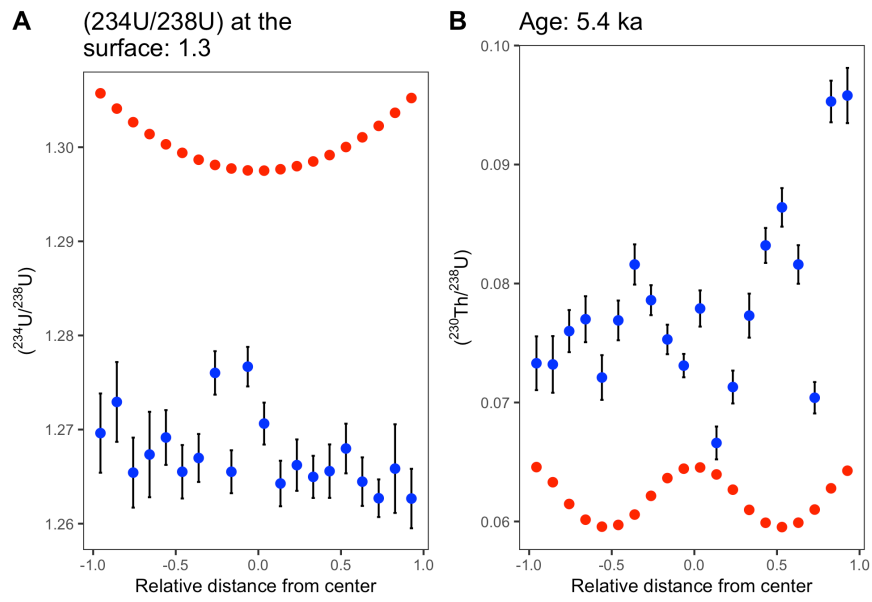


Figure 3: Results from the model's first run with the modern human femur. A: Calculated (red) and observed (blue) $(^{234}\text{U}/^{238}\text{U})$ activity ratios for transect 2 of modern human femur 132A/LB/27D/03. B: Calculated (red) and observed (blue) $(^{230}\text{Th}/^{238}\text{U})$ activity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

232 The model is thus run a second time, increasing the number of iterations to
233 1000, and changing `U48_0_min` and `U48_0_max` to 1.265 and 1.270, respectively,
234 and `T_max` to 10^3 yr. Since the first run suggests a Holocene age for the sample,
235 the measured ($^{234}\text{U}/^{238}\text{U}$) at the surfaces must be similar to the calculated
236 values, thus the chosen values for the range above.

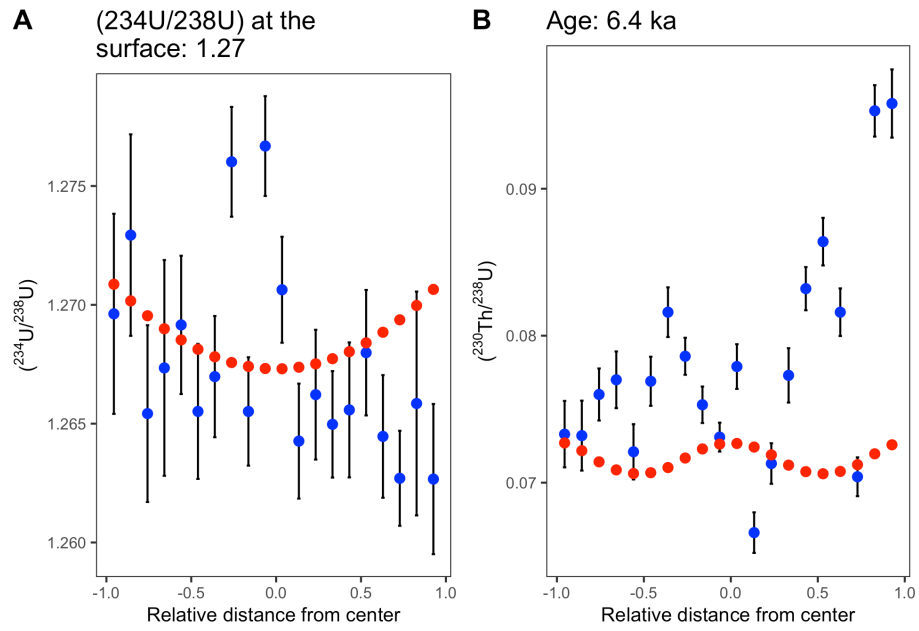


Figure 4: Results from the model's second run with the modern human femur. A: Calculated (red) and observed (blue) $(^{234}\text{U}/^{238}\text{U})$ activity ratios for transect 2 of modern human femur 132A/LB/27D/03. B: Calculated (red) and observed (blue) $(^{230}\text{Th}/^{238}\text{U})$ activity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

237 U48_0_min, U48_0_min, T_min and T_max can be further adjusted. `fsum_target`
238 can also be decreased to 0.01 in order to get a better fit and error, but it is at
239 the expense of computing time. Once a satisfying fit is obtained (assessed by
240 inspecting the figures produced), the number of iterations `nbit` can be increased
241 to 1000 (or higher). Following this method, we obtain an age of $6.4 \pm 1.4/-1.4$
242 ka (Figure 4).

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

244 For transect 1 of LB1/52, Sutikna et al. (2016) reported an age of 79.0
245 ± 3.7 ka. With iDADwigl, using data in the file `Hobbit_1-1T_for_iDAD.csv`
246 provided in the package, and following the same method as above, we obtain
247 an age of $75.4 \pm 1/-0.9$ ka (Figure 5).

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

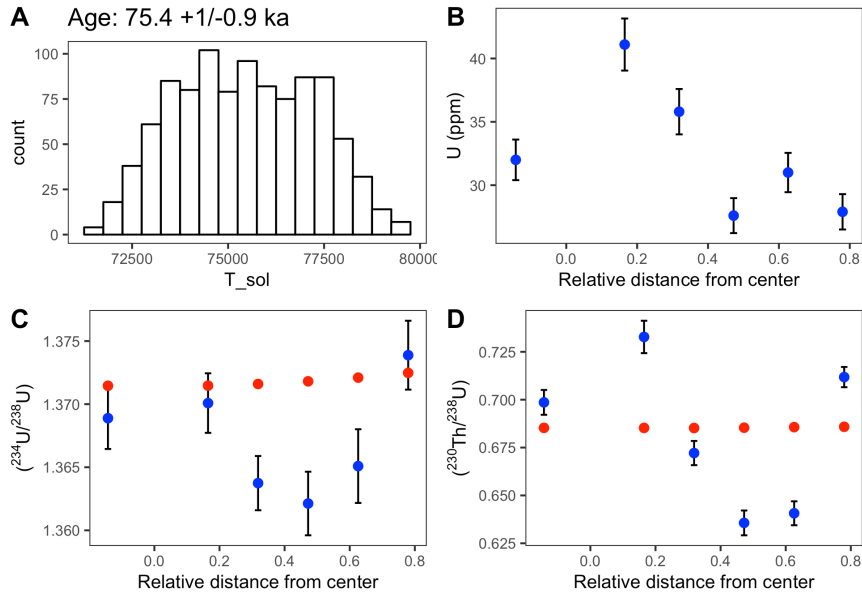


Figure 5: Results from running the model with *Homo floresiensis* ulna LB1/52 data from Sutikna et al. (2016). A: Histogram of the solution ages, B: Uranium concentration profile for transect 1 of *Homo floresiensis* ulna LB1/52. C: Calculated (red) and observed (blue) $(^{234}\text{U}/^{238}\text{U})$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

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Colophon

This report was generated on 2018-12-29 15:00:05 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 C
## ctype   en_US.UTF-8
## tz      America/Los_Angeles
## date    2018-12-29
##
## - 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]
## colorspace  1.3-2      2016-12-14 [1]
## commonmark  1.7        2018-12-01 [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]
## htmltools   0.3.6      2017-04-28 [1]
## P iDADwigl   * 0.1.0      2018-12-29 [?]
## 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]
```

```

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##      pkgconfig    2.0.2      2018-08-16 [1]
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##      processx     3.2.1      2018-12-05 [1]
##      ps           1.3.0      2018-12-21 [1]
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##      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]
##      roxygen2      6.1.1      2018-11-07 [1]
##      rprojroot    1.3-2      2018-01-03 [1]
##      rstudioapi    0.8        2018-10-02 [1]
##      rtticles     0.6        2018-10-09 [1]
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##      tidyselect   0.2.5      2018-10-11 [1]
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##      xtable       * 1.8-3      2018-08-29 [1]
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##      source
##      CRAN (R 3.5.0)
##      CRAN (R 3.5.0)
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##      Github (gaborcsardi/crayon@74bee76)
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##      CRAN (R 3.5.1)
##      CRAN (R 3.5.0)
##      Github (tidyverse/dplyr@bee3351)
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```

```

## CRAN (R 3.5.0)
## Github (tidyverse/ggplot2@7f13dfa)
## Github (tidyverse/glue@35c61e9)
## 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)
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## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
## Github (hadley/xml2@de9781d)
## CRAN (R 3.5.0)
## CRAN (R 3.5.0)
##
## [1] /Library/Frameworks/R.framework/Versions/3.5/Resources/library
##
## P -- Loaded and on-disk path mismatch.

```

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:     [3eaea69] 2018-12-29: add not-working start on a shiny app
```