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iceTEA: Tools for plotting and analysing cosmogenic-nuclide surface-exposure data from former ice margins

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# 1 iceTEA: Tools for plotting and analysing cosmogenic-nuclide surface-

#### 2 exposure data from former ice margins

3

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8

#### 9 Abstract

10 Cosmogenic-nuclide surface-exposure data provide important constraints on the 11 thickness, extent and behaviour of ice masses in the geological past. A number of online 12 calculators provide the cosmogenic nuclide community with a means of easily calculating 13 surface-exposure ages. Here we provide a platform for plotting and analysing such data. This 14 paper describes a suite of freely accessible numerical tools for visualising, evaluating and 15 correcting surface-exposure data that are used to reconstruct past glacier and ice sheet 16 geometries.

iceTEA (Tools for Exposure Ages) is available as an online interface (<u>http://ice-tea.org</u>)
and as MATLAB<sup>®</sup> code. There are 8 tools, which provide the following functionality: 1)
calculate exposure ages from <sup>10</sup>Be and <sup>26</sup>Al data, 2) plot exposure ages as kernel density
estimates and as a horizontal or vertical transect, 3) identify and remove outliers within a
dataset, 4) plot nuclide concentrations on a two-isotope diagram and as a function of depth, 5)
correct exposure ages for cover of the rock surface, 6) correct ages for changes in relative

elevation through time, and estimate 7) average and 8) continuous rates of ice margin retreat
or thinning. Three of the tools (1, 5 and 6) perform exposure age calculations, which are
based on the framework of CRONUScalc. Results are available as printed text, tables and/or
raster (.png) and vector (.eps) graphics files, depending on the tool. These tools are intended
to enable users to evaluate complex exposure histories, assess the reliability of exposure ages,
explore potential age corrections, and better analyse and understand spatial and temporal
patterns within their data.

30

31 Keywords: Glaciers and ice sheets, Be-10 and Al-26, TCN dating, Outlier test, GIA and sea

32 level, Retreat and thinning rates

33

#### 34 1. Introduction

Over the last few decades cosmogenic-nuclide surface-exposure dating has become the 35 principal approach for reconstructing past glacier and ice sheet geometries (Balco, 2011; Ivy-36 Ochs and Briner, 2014). Such research has greatly improved our understanding of global and 37 regional patterns of ice mass expansion and contraction (e.g. Hughes et al., 2016; Solomina et 38 al., 2015), centennial-scale climate events (e.g. Schaefer et al., 2009), topographic controls on 39 ice dynamics (e.g. Jones et al., 2015), and contributions of ice masses to past changes in 40 global mean sea level (e.g. Alley et al., 2005). Despite considerable advances in the 41 technique, the full potential of cosmogenic-nuclide datasets is often hindered by geologic 42 scatter, an inadequate assessment of uncertainties and/or limited user expertise in computer 43 coding for performing analyses. 44

45 Surface-exposure dating exploits the accumulation of nuclides in the Earth's surface resulting from interactions with cosmic radiation to determine the time at which a rock was 46 exposed following deglaciation (Gosse and Phillips, 2001). The exposure history can be 47 deciphered from analysis of both the nuclide concentrations and the corresponding surface-48 exposure ages in a number of ways. The pattern of burial and exposure over glacial-49 interglacial cycles can be gauged by evaluating the ratio between two different nuclides (e.g. 50 Bierman et al., 1999; Lal, 1991; Schaefer et al., 2016). The reliability of an age for a glacial 51 landform can be assessed with statistical tests such as reduced chi-squared and outlier 52 analysis of the exposure age dataset (e.g. Balco, 2011; Rinterknecht et al., 2006; Wendt and 53 Carl, 1991). Potential effects from cover of the rock surface or changes in the relative 54 elevation of the rock surface can be accounted for and tested (e.g. Cuzzone et al., 2016; 55 Schildgen et al., 2005). Rates of ice surface lowering and ice margin retreat can also be 56 estimated by quantifying the relationship between the location and exposure age of samples 57 within a dataset (e.g. Briner et al., 2009; Johnson et al., 2014). While the development of 58 online exposure age calculators (CRONUS-Earth, Balco et al., 2008; CRONUScalc, Marrero 59 et al., 2016; CREp, Martin et al., 2017) have helped facilitate the rapid growth of the 60 application, there is currently no common platform for quantitatively evaluating exposure age 61 datasets in the ways described above. 62

Here we describe iceTEA – Tools for Exposure Ages – a suite of online tools for plotting
and analysing cosmogenic-nuclide surface-exposure data that are used to constrain former ice
margins. The paper outlines the systematics of iceTEA, the basis, set up and user-inputs for
each of the tools, and it also highlights potential benefits of applying the tools to surfaceexposure datasets.

#### 69 **2. Description of the numerical tools**

#### 70 **2.1 Systematics**

The tools of iceTEA are outlined in Table 1. They can be used via an online interface (http://ice-tea.org), but are also available as MATLAB<sup>©</sup> code with an easy-to-use front-end script for each tool (see supplementary material). While the online version performs all primary analysis and plotting functionality for each tool, the code provides the user with greater flexibility to apply the tools for specific needs and also includes some additional options (e.g. selecting specific samples within the dataset to be analysed).

Tool	MATLAB <sup>©</sup> front-end script	Online stages
1. Calculate ages *	Calc_Plot_age.m	Calculation inputs Results Plot settings Plots
2. Plot ages	Import_Plot_age.m	Data input & Plot settings Plots
3. Remove outliers	Calc_Plot_age.m Import_Plot_age.m	Analysis inputs Results Plot settings Plots
4. Plot two-isotope concentrations	Plot_concs.m	Data input & Plot settings Plots
5. Correct for surface cover *	Cover_correct_ages.m	Analysis inputs Results Plot settings Plots
6. Correct for elevation change *	Cover_correct_ages.m	Analysis inputs Results Plot settings Plots
7. Estimate retreat/thinning rates - linear	Analyse_linear_rates.m	Analysis inputs Results Plot settings Plots
8. Estimate retreat/thinning rates - continuous	Analyse_continuous_rates.m	Analysis inputs Results Plot settings Plots

#### Table 1. Tools of iceTEA

\* Uses modified version of CRONUScalc calculation framework (Marrero et al., 2016).

78 Each tool is comprised of two to four stages, which include input parameters, results of the analysis, plot settings and plotted results (Table 1). iceTEA requires the details of the 79 surface-exposure dataset in a Microsoft<sup>©</sup> Excel<sup>©</sup> or comma-separated values spreadsheet, or 80 in a tab-delimited text file. The following information must be included for each sample: 81 sample name; latitude; longitude; elevation; pressure (if known); relative position (if 82 relevant); sample thickness; bulk density; shielding factor; <sup>10</sup>Be concentration (mean and 83 uncertainty, if measured); <sup>26</sup>Al concentration (mean and uncertainty, if measured); year 84 collected; and for plotting the nuclides on a two-isotope diagram, the sample depth and final 85 mineral weight (see Appendix A1). As with previous age calculators (CRONUScalc, Marrero 86 et al., 2016; CREp, Martin et al., 2017), the nuclide concentrations should be normalised to 87 07KNSTD for <sup>10</sup>Be (Nishiizumi et al., 2007) and KNSTD for <sup>26</sup>Al (Nishiizumi, 2004) before 88 89 being used with iceTEA (see

90 <u>http://hess.ess.washington.edu/math/docs/al\_be\_v22/al\_be\_docs.html</u> for details).

Four tools require exposure ages to be calculated before performing analysis and 91 plotting, while three tools involve the calculation of exposure ages. The details of each of 92 93 these tools are described in the sections below. In cases where exposure ages are already known (for example, using a different age calculator, perhaps with a local production rate), 94 the mean age, internal and/or external uncertainty and provided production rate scaling model 95 can be used (see Appendix A1). In cases where exposure ages need to be computed, a 96 modified version of the CRONUScalc calculation framework is used (see Marrero et al., 97 2016 for details). 98

Cosmogenic-nuclide production is computed for spallation, the dominant production
mechanism at the surface, and for muons, which are important at depth (Gosse and Phillips,
2001). Three principal scaling models for production by spallation can be used with iceTEA,
which have been shown to best fit production rate calibration data (Borchers et al., 2016): 1)

103	'Lm', the time-dependent version of Lal (1991), which uses variations in the dipole magnetic
104	field intensity (Nishiizumi et al., 1989); 2) 'LSD', the time-dependent model of Lifton et al.
105	(2014), which includes dipole and non-dipole magnetic field fluctuations and solar
106	modulation; and 3) 'LSDn', a version of LSD that implements nuclide-specific scaling by
107	incorporating cross-sections for the different reactions (Lifton et al., 2014). The MATLAB $^{\odot}$
108	version of iceTEA has options for other time-independent (St; Stone, 2000) and time-
109	dependent models (De, Du, Li; Desilets and Zreda, 2003; Dunai, 2000; Lifton et al., 2005).
110	The geomagnetic history used in all of the time-dependent scaling models includes the
111	CALS3k model for 0-3 ka (Korte and Constable, 2011; Korte et al., 2009), the CALS7k
112	model for 3-7 ka (Korte and Constable, 2005), the GLOPIS-75 model for 7-18 ka (Laj et al.,
113	2004), and the PADM2M model for 18-2000 ka (Ziegler et al., 2011), which is the same as
114	used in CRONUScalc. Muon flux is scaled using the energy-dependent model of Lifton et al.
115	(2014). All time-dependent scaling models are computed relative to the year that the sample
116	was collected, which is a required input for each sample. As the production rate is dependent
117	on any shielding of the rock surface (Dunne et al., 1999; Gosse and Phillips, 2001), a
118	topographic shielding factor is a required input for each sample; this can be calculated using
119	the online calculator described by Balco et al. (2008) (http://stoneage.ice-
120	d.org/math/v3/skyline_in.html), or by using the supplemental tool Topographic_shielding,
121	which is available in the MATLAB <sup>©</sup> version of iceTEA. Nuclide production is numerically
122	integrated for both time, using the selected scaling model, and the depth of the sample, based
123	on the given sample thickness (see Marrero et al., 2016). The implementation of
124	CRONUScalc within iceTEA is further described and discussed in Sections 2.2, 2.6 and 2.7.

#### 126 **2.2 Calculate ages**

127 iceTEA provides the capability to compute and plot surface-exposure ages. The primary purpose of the 'Calculate ages' tool (no. 1) is to compare the calculated ages with those ages 128 generated using correction tools (e.g. correcting for surface cover (Section 2.6) and elevation 129 change (Section 2.7)), as well as to ages derived from other calculation frameworks (e.g. the 130 online calculator formerly known as CRONUS-Earth (Balco et al., 2008), CREp (Martin et 131 al., 2017) and CRONUScalc (Marrero et al., 2016)). While the age calculations in iceTEA are 132 based on the CRONUScalc framework, exposure ages calculated using this tool may produce 133 slightly different results from CRONUScalc for a number of reasons. Firstly, atmospheric 134 pressure is calculated based on the location of each sample if it is not input by the user. The 135 ERA-40 atmospheric model (Uppala et al., 2005) is used to derive pressure, as with CREp 136 and CRONUScalc, however, an elevation-pressure relationship (Radok et al., 1996) is instead 137 138 used if the sample is from Antarctica (<-60 °S) (Balco et al., 2008; Stone, 2000). Secondly, exposures ages are calculated here assuming zero nuclide inheritance, zero surface erosion, 139 and the top depth of a sample is assumed to be the surface (zero depth). Thirdly, the effective 140 attenuation length cannot be manually set, and is instead calculated dependent on the location 141 of the sample (Sato et al., 2008); this is the same method used by CRONUScalc when the 142 attenuation length field is missing. Fourthly, uncertainty is only calculated here based on the 143 elevation and measurement errors, as well as those inherent in the production rate estimates. 144 The exclusion of additional uncertainties (e.g. associated with the bulk density, sample 145 thickness, shielding factor, attenuation length, and erosion rate) reduces computation time 146 relative to CRONUScalc by approximately a factor of four (based on tests using the St and 147 LSD scaling models). 148

Surface-exposure ages are computed using the provided input data (Section 2.1), and theoutputs can then be plotted based on the user's plotting preferences. The age distributions are

plotted as kernel density estimates, and age population statistics are calculated if the dataset is
defined as being from a single feature (described in Section 2.3). When using the MATLAB<sup>©</sup>
version, the production rate through time can also be output and plotted.

154

#### 155 **2.3 Plot ages**

The user may wish to plot and evaluate an exposure age dataset that was independently generated using a different calculation program (or previously generated with iceTEA). This tool (no. 2) allows exposure ages to be imported (as specified in Appendix A1) and then plotted.

A useful initial approach for evaluating a population of exposure ages is to look at the 160 age distribution of the dataset. Ages are plotted using this tool as kernel density estimates, 161 which are estimates for the probability density function. Details of this method are discussed 162 in Lowell (1995), however, the version here corrects for the effect in which measurements 163 with the same relative precision have shorter kernel heights - appearing less important - as 164 they get older. The probability distributions are normalised by the expected kernel heights, 165 which are calculated as a function of age, assuming that all measurements have the same 166 relative uncertainty (Balco, 2018). Exposure ages are normally distributed around the mean 167 value, and the type of uncertainty adopted depends on the dataset. External uncertainties 168 (associated with both the measurement and production rate) are used to calculate the age 169 distributions, unless the dataset is identified as being from a single 'feature' (e.g. a moraine), 170 171 when the internal uncertainties (measurement only) are instead used; for such datasets, uncertainty introduced due to differences in production rate between samples is typically 172 negligible. Individual age distributions are plotted with the summed age distribution of the 173 dataset. 174

Exposure ages from a feature should ideally represent a single age population. Statistics describing the age distribution of the dataset are calculated when 'feature' is set by the user. These include the modal age based on the summed age distribution, the weighted mean and standard deviation, and the reduced chi-squared. The weighted mean  $(\bar{\mu})$  and weighted standard deviation  $(\bar{\sigma})$  of the dataset are calculated as:

180 
$$\bar{\mu} = \sum_{i} \left( \frac{1/v_i}{\sum_i 1/v_i} \right) x_i \tag{1}$$

181 and

182 
$$\bar{\sigma} = \sqrt{\sum_{i} \left(\frac{1/v_i}{\sum_{i} 1/v_i}\right) (x_i - \bar{\mu})^2} \tag{2}$$

183 where  $v_i$  is a sample's analytical age uncertainty and  $x_i$  is a sample's mean age. If preferred, 184 it is possible to alternatively calculate the arithmetic (unweighted) mean and standard 185 deviation (MATLAB<sup>©</sup> version only). The reduced chi-squared ( $\chi_R^2$ ) – often referred to as the 186 mean square of the weighted deviations (MSWD) in some areas of geochronology (e.g. 187 Wendt and Carl, 1991) – is a measure of the goodness of fit between the weighted mean and 188 the set of exposure ages. It is calculated as follows:

189 
$$\chi_R^2 = \frac{1}{n-1} \sum_{i=1}^n \frac{(x_i - \overline{\mu})^2}{v_i^2}$$
 (3)

190 where the degrees of freedom is one less than the number of samples (*n*). A  $\chi_R^2$  value of 191 approximately 1 signifies that the scatter in the dataset can be explained by the measurement 192 uncertainty of the individual samples alone, producing a univariate normal distribution where 193 the weighted mean and uncertainty appropriately represent the data. The measurement 194 uncertainties may have been overestimated if the value is significantly less than 1. For values 195 larger than 1, the observed scatter of the data exceeds that predicted by the age uncertainties, 196 indicating an additional source for variance in the data, most likely from geomorphic factors.

197 To test whether the data represent a single feature, a reduced chi-squared value should fall 198 within a  $2\sigma$  envelope (95% confidence), determined by the criterion  $\kappa$ :

199 
$$\kappa = 1 + 2\sqrt{\frac{2}{n-1}}$$
 (4)

which depends on the degrees of freedom and, therefore, the number of samples (Spencer et al., 2017; Wendt and Carl, 1991). If  $\chi_R^2 < \kappa$  then there is a >95% probability that the data represent a single population and it is therefore appropriate to use the weighted mean as an age estimate for the feature (Spencer et al., 2017). A thorough evaluation of a dataset from a single feature should also attempt to identify outliers, which uses different statistical methods (see Section 2.4).

For spatially-variable datasets where samples have been collected at a range of locations relative to an ice margin, it is informative to show exposure ages as a function of their sample position. If the dataset is identified by the user as a 'transect', then exposure ages are additionally plotted as either a vertical or horizontal transect. The relative position is used from the input data (Appendix A1), which should be in metres for a vertical transect and km for a horizontal transect. If there are no relative position values entered for samples from a vertical transect, then the elevation (in metres above sea level) is used.

A series of plotting options are available. The user can set the time axis limits (lower and upper) in thousands of years before present (ka), and position axis limits (lower and upper) in metres or km depending on the type of relative position data (applies only to the transect plot). In the MATLAB<sup>©</sup> version, particular samples within the dataset can be selected to plot (the default is to plot all samples given in the input data).

#### 219 **2.4 Remove outliers**

Glacial chronologies often have a degree of scatter where samples do not provide 220 matching exposure ages. For glacial features, such as moraines or bedrock landforms, a suite 221 of samples is typically collected to provide an accurate age constraint. While the shape of a 222 summed probability distribution can be used to indicate potential outliers – a single discrete 223 peak implies all ages with uncertainties are consistent with each other, more than one discrete 224 peak implies no single consistent age population, and a peak with a shoulder peak on one of 225 its limbs implies something in between – it is partially subjective. To more robustly identify 226 whether a dataset represents a single age population or a dominant age population and an 227 outlier, statistical outlier tests like the Chauvenet's criterion (e.g. Rinterknecht et al., 2006) 228 and Grubbs' Test (e.g. Putnam et al., 2010), and assessments of dataset skewness (Applegate 229 et al., 2010) have been applied. 230

In this tool (no. 3) we use a two-tailed generalised extreme Studentized deviate (gESD) 231 232 test to statistically identify whether there are any outliers within the dataset (Rosner, 1983). Similar to the Grubbs' Test (Grubbs, 1969), it assumes that the data can be approximated by a 233 normal distribution, and is performed iteratively using the difference between the sample's 234 mean exposure age and the most extreme data considering the standard deviation. Unlike the 235 Grubbs' Test, the gESD test does not assume a single outlier, and instead uses an upper 236 bound for the number of possible outliers (r). The outliers are calculated from a sequence of 237 separate tests (1 outlier, 2 outliers, ..., r outliers): 238

239 
$$R_i = \frac{|x^{(i)} - \bar{x}^{(i)}|}{s^{(i)}}$$
(5)

where  $R_i$  is Rosner's test statistic representing the extreme Studentized deviates from successively reduced samples,  $x^{(i)}$  is the observation with the greatest distance from the

mean of the dataset, and  $\bar{x}^{(i)}$  and  $s^{(i)}$  are the mean and standard deviation of the dataset with the most extreme observations removed. Critical values ( $\lambda_i$ ) for  $R_i$  are calculated as:

244 
$$\lambda_i = \frac{t_{p,n-i-1}(n-i)}{\sqrt{(n-i-1+t_{p,n-i-1})(n-i+1)}}$$
 (6)

where *n* is the number of observations,  $t_p$  is the Student's t-distribution for the quantile of significance level  $\alpha$  (the default is 0.05; 5% probability of incorrectly rejecting the null hypothesis that there are no outliers), and n - i - 1 determines the degrees of freedom.

The number of outliers is determined by finding the iteration with the most successively 248 reduced samples (the largest *i*). If  $R_i > \lambda_i$  then the *i* most extreme values are outliers. We set 249 the maximum number of outliers (r) as n - 1; by assuming a high number of possible 250 outliers, we avoid additional outliers influencing the value of the test statistic. The method is 251 most accurate for datasets with at least 15 samples, and particularly >25 samples (Rosner, 252 1983). Datasets with fewer samples require there to be much fewer outliers for accurate 253 detection. For example, at the most extreme, no more than a single outlier could be reliably 254 identified from a dataset of only 3 samples. 255

The outlier identification and removal tool is featured differently in the online and 256 MATLAB<sup>©</sup> versions of iceTEA. The tool is included within the age calculation and plotting 257 tools (Sections 2.2 and 2.3) in the MATLAB<sup>©</sup> version (Table 1). On the web interface it is a 258 separate tool, requiring sample exposure ages to be calculated and included in the input 259 sample data (Appendix A1). By using the tool, it is assumed that the data come from a single 260 feature (e.g. a moraine or bedrock landform), and that there should be a consistent age 261 population for that feature. If a dataset contains multiple features, then the analysis must be 262 performed separately for each feature, with the input data organised accordingly. For a more 263 thorough assessment of a dataset, the significance level for determining outliers ( $\alpha$ ) can be 264

265 optionally set to 0.01 (default is 0.05), which would instead generate results with a 1% probability of incorrectly rejecting the null hypothesis that there are no outliers. Once the 266 outliers have been identified and removed, the reduced dataset of the feature is plotted as a 267 kernel density plot with the corresponding modal age, weighted mean and standard deviation, 268 and reduced chi-squared statistic (as in Section 2.3). The removed outliers can optionally be 269 plotted as grey kernel density estimates. If no outliers are detected then this plot will contain 270 all original ages within the dataset. The user can optionally set the time axis limits (lower and 271 upper) of the plot in thousands of years before present (ka), and specify which samples to plot 272 (MATLAB<sup>©</sup> version only). 273

274

#### 275 **2.5 Plot two-isotope concentrations**

Multiple nuclides (most commonly <sup>10</sup>Be and <sup>26</sup>Al) are often measured in a sample to 276 better understand the exposure and burial history (Lal, 1991), and can be particularly useful 277 in burial dating and for identifying cosmogenic inheritance in a sample (e.g. Fabel and 278 Harbor, 1999; Granger, 2006). The 'Plot two-isotope concentrations' tool (no. 4) enables 279 measured nuclide concentrations to be plotted on a two-isotope diagram and optionally as a 280 depth profile, using the information provided in the input data. It should be noted that the 281 required data are slightly different from that needed for the other tools (see Section 2.1 and 282 Appendix A1). The tool is currently only available for <sup>10</sup>Be and <sup>26</sup>Al data. 283

The purpose of a two-isotope diagram is to compare measured nuclide concentrations with those concentrations that should be expected from simple pathways of exposure and burial (Figure 1). The concentration of a nuclide ( $N_k$ ) during exposure differs between isotopes, owing to nuclide-specific production and decay:

288 
$$N_{k} = \frac{P_{k}}{\lambda_{k} + \frac{\rho\varepsilon}{\Lambda}} \left( 1 - exp\left[ -\left(\lambda_{k} + \frac{\rho\varepsilon}{\Lambda}\right) \right] t_{e} \right)$$

where  $P_k$  is the nuclide's production rate (atoms  $g^{-1} a^{-1}$ ),  $\lambda_k$  is the nuclide's decay constant 289 (a),  $\rho$  is rock density (g cm<sup>-3</sup>),  $\varepsilon$  is the surface erosion rate (cm a<sup>-1</sup>),  $\Lambda$  is the attenuation length 290  $(g \text{ cm}^{-2})$ , and  $t_e$  is the exposure time (a). For a continuously exposed rock surface, the 291 concentration of <sup>10</sup>Be increases until it reaches secular equilibrium, while the ratio of <sup>26</sup>Al to 292 <sup>10</sup>Be decreases as the lower half-life of <sup>26</sup>Al causes it reach secular equilibrium sooner (top 293 curve in Figure 1). A rock surface can experience different concentration pathways despite 294 continuous exposure as a result of subaerial erosion. A second, lower curve is determined by 295 calculating nuclide saturation from continuous exposure and a multitude of erosion rates. A 296 steady-state erosion island (Lal, 1991) - referred to here as the "simple exposure region" -297 represents the area within which a continuously exposed surface can exist (Figure 1). 298 Following exposure, when a surface becomes buried and protected from cosmic rays, the 299 concentration of <sup>26</sup>Al decays more quickly than that of <sup>10</sup>Be; the <sup>26</sup>Al/<sup>10</sup>Be ratio decreases in 300 301 line with radioactive decay. Exposure and burial isochrones, representing concentrations of equal exposure  $(t_e)$  and burial  $(t_b)$  time (a), are plotted on the diagram and calculated with: 302

303 
$$N_{k} = \frac{P_{k}}{\lambda_{k} + \frac{\rho}{\Lambda}} \left( 1 - exp\left[ -\left(\lambda_{k} + \frac{\rho}{\Lambda}\right) \right] t_{e} \right) exp\left[ -\left(\lambda_{k} + \frac{\rho}{\Lambda}\right) \right] t_{b}$$
(8)

where it is assumed that the surface is buried at an infinite depth, with zero production, following initial continuous exposure rather than steady-state erosion. The diagram (Figure 1) assumes that a sample has primarily experienced spallogenic production, at or near to the surface, rather than muonic production at greater depths. In situations where a sample underwent significantly more production at depth (i.e. below ~5 m) than at the surface – for fast-eroding settings and/or deep cores – the ratio between <sup>26</sup>Al and <sup>10</sup>Be would be greater

310 (e.g. Akçar et al., 2017; Granger and Smith, 2000) and the sample would appear further up

#### the diagram (Fig. 1).

#### 312





329 To allow for comparing samples from multiple sites, it is necessary to normalise nuclide concentrations. A depth-integrated local present-day production rate of each sample is 330 calculated and averaged by the mineral weight, while the mean density and attenuation length 331 of the samples are used to compute the exposure and burial isochrones and lines of 332 continuous exposure. As the nuclide concentrations are normalised by the nuclide's 333 production rate,  $P_k$  in Equations 7 and 8 becomes equal to 1. 334 The plot can also be produced for nuclide concentrations from core samples, where some 335 samples may have been combined for a nuclide measurement. An example is where, at a 336 particular depth range, two samples were independently measured for <sup>10</sup>Be but were 337

combined for <sup>26</sup>Al measurement (e.g. Schaefer et al., 2016). Based on the sample input data (see Section 2.1 and Appendix A1), data are automatically sorted by finding common depths between nuclide measurements and then combining the normalised concentration means ( $\hat{N}_c$ ) and uncertainties ( $\hat{\sigma N}_c$ ) for the depth range:

342 
$$\widehat{N}_c = \frac{\sum_c (\widehat{N}_s \sum w_s)}{\sum_c (\sum w_s)}$$
(9)

343 and

344 
$$\widehat{\sigma N}_c = \sqrt{\left(\frac{\sum_c (\widehat{N}_s \sum w_s)}{\sum_c (\sum w_s)}\right)^2}$$
(10)

where  $\hat{N}_s$  is the normalised sample concentration (with the unit being years, as the concentration is normalised by the production rate) and  $w_s$  is the weight of each sample (g). The two-isotope diagram uses a logarithmic axis for the normalised <sup>10</sup>Be concentration (Nishiizumi et al., 1991) as 1) it reduces clustering of samples, particularly for low <sup>10</sup>Be concentrations, and 2) radioactive decay lines and corresponding burial isochrones are nearstraight, allowing for simpler interpretation of data with respect to time. Sample

351	concentrations are plotted with uncertainty ellipses and a point mean. The ellipses can be
352	shown for either 1 or 2 $\sigma$ (68% or 95% confidence). The user can also optionally set the
353	<sup>26</sup> Al/ <sup>10</sup> Be ratio and <sup>10</sup> Be concentration axes limits (lower and upper) and, in the MATLAB <sup>©</sup>
354	version, set the exposure and burial isochrones (in ka) to plot.

Depth profiles can be particularly useful for evaluating nuclide production in soils and bedrock (e.g. Balco and Rovey, 2008; Schaefer et al., 2016). This tool provides the option to additionally plot sample concentrations (in atoms  $g^{-1}$ ) as a function of depth (m), where a box represents the depth range and the concentration uncertainty of each sample, and a line represents the mean concentration for that sample. The depth and concentration axes limits (lower and upper) can be optionally set when producing this plot using the MATLAB<sup>©</sup> version.

362

#### 363 **2.6 Correct for surface cover**

Cosmogenic nuclide production in rock decreases with depth below the surface as 364 cosmic radiation is attenuated. The same process occurs in material overlying the rock 365 surface – dependent on the thickness and density of that material – which can shield the rock 366 surface from cosmic rays and therefore reduce nuclide production (Gosse and Phillips, 2001). 367 The effects of shielding from surface cover are commonly ignored or considered negligible, 368 but feasible depths of >16 g cm<sup>-2</sup> reduce nuclide production by >10%. Two main approaches 369 370 can be taken if a study region is suspected to have had some surface cover (e.g. snowpack, 371 soil, loess, till, ash, water): 1) a specific sampling strategy to minimise the effects of possible surface cover – for example, only the top surfaces of large boulders could be sampled, 372 373 assuming that these would not have been covered or that any material was quickly windswept 374 (e.g. Balco, 2011; Ivy-Ochs et al., 1999); or 2) the influence of surface cover on collected

375 rock samples could be evaluated by calculating surface cover shielding factors and resulting
376 exposure ages (e.g. Benson et al., 2004; Schildgen et al., 2005).

Here we provide a tool (no. 5) that calculates exposure ages with a correction for material

378 covering the rock surface. The total time-averaged surface shielding factor  $(S_S)$  is calculated

379 from:

$$380 S_S = S_T \exp\left(-\frac{z_{cover}\,\rho_{cover}}{\Lambda_S}\right) (11)$$

where  $S_T$  is the shielding factor from topography (Dunne et al., 1999), and where shielding 381 from surface cover is determined from the average depth of surface cover ( $z_{cover}$ , in cm), the 382 average density of that cover ( $\rho_{cover}$ , in g cm<sup>-3</sup>) and the effective attenuation length ( $\Lambda_s$ , in g 383  $cm^{-2}$ ). The topographic shielding factor is taken from the sample input data (see Section 2.1), 384 while the attenuation length is determined from the sample location (see Section 2.2). A value 385 386 for cover depth is required, as well as either a preset cover type (Table 2) or a manually specified density for the surface cover. Exposure ages are then calculated as described in 387 Marrero et al. (2016) and Section 2.2 388

**Table 2.** Preset cover material options and the corresponding density ( $\rho_{cover}$ ) used for surface cover corrections. A user-specified density for surface cover can alternatively be used.

surface cover can alternatively be used.	
Cover material	Density (g cm <sup>-3</sup> )
Ash	0.7
Loess	1.6
Snow	0.27
Soil	1.3 <sup>a</sup>
Till	1.8
Fresh water	0.999 <sup>b</sup>
Sea water	1.027 <sup>c</sup>

<sup>a</sup> Average of dry mineral soil (~1–1.6 g cm<sup>-3</sup>); note, a value for wet soil will be higher.

<sup>b</sup> Near-surface water (1.1 bars) at 10 °C.

 $^{\rm c}$  Near-surface water (1.1 bars) at 10  $^{\rm c}C$  with salinity of 35 g kg  $^{\rm 1}$  .

390 The cover shielding factor computed in this tool is a simplified approach to be used to test the effects from long-term averages of surface cover, as it assumes that surface cover was 391 of constant depth for the entire period of interest. In reality, snow cover at a site likely varied 392 393 through time with seasonal fluctuations, water levels could have varied periodically or lowered progressively, and till, soil, loess and ash-type deposits may have gradually deflated 394 over time. In locations where snow cover was likely prevalent, there are methods available 395 that use seasonal changes in snow-depth (Gosse and Phillips, 2001), or an energy balance 396 model to account for temporal and spatial variability of snow shielding (Schildgen et al., 397 398 2005). Ideally, corrected exposure ages should use a time-dependent shielding factor, however this requires estimates of the cover depth (and density) through time, which is rarely 399 possible to approximate. It should also be noted that a more complex mass-shielding 400 approach is possibly required to accurately account for production from thermal neutron 401 capture (Delunel et al., 2014; Dunai et al., 2014; Zweck et al., 2013) and for variations in 402 cover density with depth (Jonas et al., 2009). 403

Results are provided following computation of the shielding factor and corresponding
exposure ages for the specified production scaling method. These results include the surface
cover and total shielding factors, and the corrected surface-exposure ages (mean and standard
deviation). The corrected age distributions are plotted as kernel density estimates (described
in Section 2.3).

409

410 **2.7 Correct for elevation change** 

Cosmogenic nuclide production is dependent on atmospheric pressure, with greater
production occurring at higher altitudes where the pressure is lower (Gosse and Phillips,
2001; Lal, 1991). An accurate estimate of the atmospheric pressure during exposure is,

414 therefore, necessary for the calculation of an exposure age. Typically, it is assumed that the elevation of a sampled surface relative to sea level – the reference point for scaling 415 atmospheric pressure – has either not varied over time or that any effect of elevation change 416 is negligible. However, while atmospheric pressure at present-day sea level was likely similar 417 to today in the past (Mélières et al., 1991), we know from models of glacial isostatic 418 adjustment (GIA) (e.g. Peltier et al., 2015) that vertical deformation of the land varied over 419 time in response to changing volumes of ice masses. Where a surface-exposure dating site is 420 located next to the coast, a relative sea-level curve has previously been used to estimate 421 relative changes in elevation since ice retreated from that region (e.g. Goehring et al., 2012; 422 Rinterknecht et al., 2006; Young et al., 2013). Away from the coast and relative sea-level 423 sites, it is not possible to accurately extrapolate any recorded elevation changes, largely 424 because the local ice loading history and resulting glacial isostatic response vary in space (cf. 425 Whitehouse, 2018). In such cases, GIA models can be used to derive exposure ages that are 426 corrected for isostatic change (e.g. Cuzzone et al., 2016; Suganuma et al., 2014; Ullman et 427 al., 2016). Tectonically-driven elevation change will also have an effect on nuclide 428 production (Dunai, 2010; Riihimaki and Libarkin, 2007). Rock samples that have been 429 exposed over long timescales, or that are from areas of rapid uplift/subsidence, may therefore 430 also require correction of local production rates and resulting exposure ages (e.g. Brook et al., 431 1995; Dunai et al., 2005; Schaefer et al., 1999). 432

In this tool (no. 6), exposure ages are calculated with corrections for changes in elevation
- derived from either a GIA model or a linear rate (uplift or subsidence) – through time. The
time-varying (*t*) elevation relative to present-day sea level (*E*) is determined from:

436  $E_m(t) = e_{pres,m} + e_{diff,m}(t)$ 

437 (12)

438 where  $e_{pres,m}$  is the present-day elevation (m asl) of a sample (m), and  $e_{diff,m}(t)$  is the 439 elevation (metres) of a sample relative to  $e_{pres,m}$  at time t. For a given rate (m ka<sup>-1</sup>), 440  $e_{diff,m}(t)$  is computed back to 8160 ka before present (approx. 6 times the half-life of <sup>10</sup>Be) 441 in 100-year intervals. Using a GIA-derived correction,  $e_{diff,m}(t)$  is the past isostatic 442 elevation change, interpolated from model output at 100-year intervals.  $E_m(t)$  is then 443 converted to atmospheric pressure, dependent on its location (see Section 2.2). The total 444 nuclide production is calculated based on the corrected atmospheric pressure (p):

445 
$$P_{total,k}(t) = S_{el,\zeta}(p, R_c, t) S_S P_{ref,S,\zeta,k} \exp\left(\frac{-z}{\Lambda_s}\right) + S_S P_{\mu}(p, R_c, z)$$
(13)

where  $S_{el,\zeta}$  is the time-dependent elevation-latitude scaling factor for a particular scaling 446 model ( $\zeta$ ),  $S_S$  is the shielding factor from terrain and surface cover (see Section 2.6),  $P_{ref,s,\zeta}$ 447 is the reference spallogenic (s) production rate (atom  $g^{-1} a^{-1}$ ) at present-day sea-level high-448 latitude (where p = 1013.25) for nuclide k,  $\Lambda_s$  is the effective attenuation length (g cm<sup>-2</sup>), z 449 is the depth (g cm<sup>-2</sup>), and  $P_{\mu}$  is the production rate (atom g<sup>-1</sup> a<sup>-1</sup>) at z due to muons ( $\mu$ ), which 450 is a function of pressure, depth and the cutoff rigidity  $(R_c)$ . Applying a GIA-based correction 451 to the primary <sup>10</sup>Be calibration sites of Borchers et al. (2016) increases the time- and site-452 averaged production rate by just 0.17% (based on the ICE-6G ice model and LSD scaling 453 model), well within the uncertainty of the measurements and calculation (Jones et al., in 454 review). The reason for only a minor correction is largely because the sites were far enough 455 away from the centres of past major glacial isostatic change. For long-term subsidence or 456 uplift, it can be assumed that effects were region-specific and did not influence production at 457 the calibration sites. We therefore use the uncorrected spallogenic production rate of 458 459 Borchers et al. (2016) for calculating exposure ages that are corrected for changes in relative elevation. 460

461	Determination of the time-dependent relative elevation of a sample $(e_{diff,m}(t))$ requires
462	particular inputs based on whether the GIA model or linear rate approach is used. For the
463	linear rate method, a rate of elevation change (m ka <sup>-1</sup> ) is required to generate an elevation
464	history. A positive rate (e.g. 2 m ka <sup>-1</sup> ) would correspond to lower elevations in the past,
465	uplifting towards present, and a negative rate would correspond to higher elevations in the
466	past, subsiding towards present. For the GIA-based method, either the ICE-5G (Peltier, 2004)
467	or ICE-6G (Peltier et al., 2015) ice model can be selected, which are the only global ice
468	models currently freely available. Most ice masses are included in these models (Antarctica,
469	Greenland, Laurentide, Cordilleran, Fennoscandian, British-Irish, Patagonian, New Zealand,
470	and Iceland), but the relatively minor effects from ice in the Himalayas, European Alps,
471	Caucasus and Andes do not feature. There are some differences between the ice models,
472	particularly in North America, but ICE-6G is considered to be more accurate as it is
473	constrained by modern GPS-measured uplift rates in addition to ice extent and relative sea-
474	level records. The original ice model data was also produced for different timescales, with
475	ICE-5G ice history defined from 122 ka to present, but ICE-6G from just 26 ka. Prior to these
476	times, the elevation difference for the oldest model time step is used and, therefore, corrected
477	exposure ages older than 122 ka or 26 ka should not be interpreted.

In addition to defining the ice-load history, the rheological properties of the Earth must 478 be prescribed within the GIA model. A three-layer approximation of the VM2 Earth model 479 480 (5G reference) is used in our calculations. The VM2 Earth model was developed in conjunction with the ICE-5G ice model, while the ICE-6G ice model was developed in 481 parallel with the VM5a Earth model (6G reference). VM5a is simply a multi-layer fit to 482 483 VM2, so our 3-layer approximation is appropriate for use with both ice models. Having defined both the ice model and the Earth model, the time-dependent elevation relative to 484 present can be calculated. The spatial resolution of the GIA model output used within iceTEA 485

is 1 geographic degree, meaning that a greater spatial variability of isostatic effects is
captured towards the poles. The GIA model accounts for shoreline migration, rotational
feedbacks, and the gravitational attraction of ice masses (Milne and Mitrovica, 1998;
Whitehouse, 2018). If the sample elevation is below sea level for any particular period of
time, then it is assumed that no nuclide production occurs.

Results are provided following computation of the time-dependent elevation and 491 corresponding exposure ages for the specified production scaling method. These results 492 include the corrected surface-exposure ages (mean and standard deviation) and the mean 493 offsets from the uncorrected ages (in years and as a percentage), which are exported as an 494 Excel<sup>©</sup> spreadsheet or text file. The corrected age distributions are plotted as kernel density 495 estimates (described in Section 2.3), and the local production rates used are plotted as a 496 function of time. The age axes of the plots, as well as the production rate axis, can be 497 498 optionally set (lower limit and upper limit).

499

# 500 2.8 Estimate retreat/thinning rate – linear approach

Surface-exposure dating is sometimes applied in transects to constrain spatial changes of 501 the ice margin through time (e.g. Briner et al., 2009; Cuzzone et al., 2016; Johnson et al., 502 2014; Lane et al., 2014; Small et al., 2018). Linear rates of deglaciation can then be estimated 503 by either calculating the distance and age offset between dated positions, or by performing 504 regression analysis for a suite of exposure ages that vary approximately linearly with their 505 506 position. The latter approach has been used to derive average rates and corresponding durations of rapid ice surface lowering in Antarctica (Johnson et al., 2014; Jones et al., 2015; 507 Small et al., accepted), and is adopted here (tool no. 7). 508

Ice margin retreat or thinning rate estimates are computed for datasets that form either a horizontal or vertical transect, respectively. The positions of the samples relative to the ice margin (in km for horizontal transects and metres for vertical transects) are used as the independent variable in the analysis. Least-squares regression is applied randomly to normally-distributed exposure ages (at 2  $\sigma$ ) through a Monte Carlo simulation; while 5000 is the default number of iterations, this value can be optionally specified. Linear least-squares regression predicts the exposure age ( $y_i$ ) for each sample position regressor ( $q_i$ ):

516  $y_i = \beta_0 + \beta_1 q_i \tag{14}$ 

517 where  $\beta_1$  is the Pearson correlation coefficient of the observed mean exposure ages and 518 sample positions, multiplied by the standard deviation of the mean ages divided by the 519 standard deviation of the positions, and  $\beta_0$  is the mean of the observed ages minus the mean 520 of the observed sample positions multiplied by  $\beta_1$ .

521 The approach assumes that 1) the exposure ages accurately represent the timing of ice margin retreat or ice surface lowering at each position, without any post-depositional 522 processes or cosmogenic inheritance significantly affecting the ages, and 2) retreat/thinning 523 was approximately continuous over the time period. Rates are estimated from the distribution 524 of feasible, positive-sloping linear regressions. The uncertainty of the estimate is generally 525 reflective of the number and scatter of exposures ages contributing to each transect, together 526 with their respective uncertainties. Uncertainties in the horizontal/vertical positions of 527 samples are not included in the calculations. 528

Linear estimates can be computed using either unweighted or weighted regression, where the weighting is derived from the analytical uncertainty of each sample (see Equations 1 and 2). While the weighted method should be used if some of the exposure ages have large uncertainties relative to others in the dataset, the unweighted method should be used if

outliers within the data are suspected, particularly if those potential outliers have relativelysmall uncertainties.

535	The computed linear rates are produced as a probability distribution, with estimates at
536	68% and 95% confidence bounds. Estimated rates are plotted as a histogram, highlighting the
537	modal and median rate, and as a transect, showing all modelled linear regressions for the
538	exposure ages as a function of sample position. For the latter plot, the user can specify
539	whether to show the exposure ages, and can optionally set the time and relative position axes
540	(lower and upper limits) in thousands of years before present and in metres or km,
541	respectively. In the MATLAB <sup><math>^{\circ}</math></sup> version, the samples to be analysed within the dataset can
542	also be specified (the default is to analyse all samples).

543

#### 544 **2.9 Estimate retreat/thinning rates – continuous approach**

A surface-exposure dataset may record a variable rate of ice retreat or thinning during deglaciation (e.g. Lane et al., 2014; Spector et al., 2017). In this case an average rate derived from a linear regression model (Section 2.8) will not adequately capture the ice margin or ice surface elevation changes implied by the data. Alternatively, the continuous evolution of such changes can be modelled to derive rate estimates, enabling the magnitude and timing of rate changes to be identified and datasets from different locations to be compared (e.g. Cahill et al., 2015).

Here we provide a tool (no. 8) that estimates rates of retreat or thinning by fitting a
continuous time-dependent function of ice position with respect to time. The relative position
(distance from ice margin or elevation above the modern ice surface) is modelled using
Fourier Series analysis:

556 
$$f(t) = a_0 + \sum_{i=1}^n a_i \cos(wti) + b_i \sin(wti)$$

where f(t) is the true relative sample position under the assumptions of the fitted model, t is 557 the mean age of the mean sample position,  $a_i$  and  $b_i$  are coefficients for the cosine and sine 558 forms, w is the frequency of the signal, and i is the number of terms in the series. The latter 559 of these parameters can be optionally modified to manually improve the fit of the model to 560 the data (values are accepted between 1 and 8; default is 3); the higher the number of terms 561 (*i*), the more sinusoidal the fit. While potentially useful, this is a simple approach that 1) uses 562 only the mean exposure age and position values, 2) may assume that the exposure ages can 563 record retreat/thinning and advance/thickening, and 3) requires the user to decide which 564 model (determined by the number of terms) best fits the data. 565

The MATLAB<sup>©</sup> version of iceTEA includes an additional, more robust statistical approach,
designed for surface-exposure data. In this case, the relative position is modelled using
Bayesian penalized spline regression:

569 
$$f(t_i) = \sum_{k=1}^{K} b_k(t) \alpha_k$$
 (16)

where  $t_i$  is the age of the sample position and  $f(t_i)$  is the true relative position under the 570 assumptions of the fitted model,  $\alpha_k$  refers to spline coefficient k and  $b_k$  is the  $k^{th}$  B-spline 571 evaluated at age t, for k = 1, ..., K. Cubic B-splines (e.g. Eilers and Marx, 2010) were used 572 and the first order differences of the spline coefficients were penalized to ensure smoothness 573 of the fitted curve. As surface-exposure dating assumes continuous deglaciation without 574 readvance or re-thickening, a further constraint was imposed on the coefficients so that the 575 spline-modelled positions decreased over time. The model was fitted within a Bayesian 576 577 framework using JAGS (just another Gibbs sampler; Plummer, 2003) to provide estimates of  $f(t_i)$  with uncertainties, which were incorporated through an errors-in-variables framework 578 (Cahill et al., 2015; Dev et al., 2000). For a vertical transect, both temporal (exposure age) 579

and spatial (elevation) uncertainties are included, while just the exposure age uncertainty isused for a horizontal transect.

Computed time-dependent estimates are produced for the median, and 68% and 95% 582 confidence bounds. The fitted age-position profile is plotted together with the rates of change 583 as a function of time, and the minimum and maximum median rates are identified and 584 highlighted. The user can specify whether to show the exposure ages, and can optionally set 585 the time, relative position and rate of change axes (lower and upper limits) in thousands of 586 vears before present, in metres or km, and in cm yr<sup>-1</sup> or m yr<sup>-1</sup>, respectively. In the 587 MATLAB<sup>©</sup> version, the samples to be analysed within the dataset can be specified (the 588 default is to analyse all samples), and the number of Monte Carlo iterations within the 589 Bayesian framework can be set (the default is 20,000). 590

591

#### 592 **3. Example applications and outputs**

The iceTEA tools can be used for most <sup>10</sup>Be and <sup>26</sup>Al surface-exposure datasets that are used to constrain former ice margins, but the choice of tool depends on the context of the dataset. Each of the tools plot nuclide concentrations, exposure ages, and/or results of an analysis, which are available for download using the online interface or can be automatically saved using the MATLAB<sup>©</sup> code, in both raster-based Portable Network Graphics (.png) and vector-based Encapsulated Postscript (.eps) formats. This section highlights potential applications for each of the tools and provides overviews for the graphical outputs of iceTEA.

600 The duration and nature of past ice cover can be apparent from nuclide concentrations 601 alone, without the need for calculating corresponding exposure ages. Rock samples that have 602 paired <sup>10</sup>Be and <sup>26</sup>Al measurements can be evaluated with the 'Plot two-isotope

603 concentrations' tool (no. 4) (Figure 2). Measured nuclide concentrations that plot within the simple exposure region likely record continuous exposure since first exposed, while 604 concentrations that plot below this area indicate that the sample underwent at least one period 605 of burial since first exposed. In Figure 2A, the measured concentrations from a Greenland 606 bedrock core (Schaefer et al., 2016) – corresponding to core segments at 0.22-0.99 m and 607 1.02-1.29 m (Figure 2B) – imply at least ~25-50 ka of exposure and ~700-1600 ka of burial. 608 Such applications can help reveal the relative duration of past ice cover and whether the 609 landscape was covered by cold-based, non-erosive ice (e.g. Briner et al., 2006), but can also 610 611 be combined with numerical modelling approaches to identify potential glacial/interglacial scenarios (e.g. Schaefer et al., 2016). 612



Fig. 2. Nuclide concentrations plotted A) on a two-isotope diagram (at 1 and 2 sigma), and B) as a
function of depth (at 1 sigma). These are examples produced by the tool 'Plot two-isotope
concentrations', which reproduce previously published plots of <sup>10</sup>Be (red) and <sup>26</sup>Al (blue) nuclide
concentrations that were measured in a bedrock core (Schaefer et al., 2016). In this case, those core
segments that were combined for nuclide measurement are automatically detected based on common
sample depths (linked with a vertical line through the means in B) in order to produce the equivalent
<sup>10</sup>Be and <sup>26</sup>Al nuclide concentrations that are shown in A. It is unlikely that samples would be

622 combined for surface rock samples, and therefore each sample would be plotted on the two-isotope623 plot separately.

624

Most of the plotting and analysis tools are for use with surface-exposure ages. The 625 overall distribution of ages within a dataset can be visualised with a kernel density plot, using 626 either the 'Calculate ages' or 'Plot ages' tool (no. 1 and 2, respectively). For a 627 geographically-distributed dataset (e.g. sequence of moraines, isolated bedrock features or 628 glacial deposits), temporal patterns in the chronology such as those across a region of New 629 Zealand can be identified (Figure 3A). It should be noted, however, that such an application 630 would have to assume that none of the exposure ages were biased by post-depositional 631 disturbance or inheritance of nuclides from prior exposure, making an apparent age younger 632 or older respectively. For datasets from a vertical or horizontal transect, patterns of ice 633 surface lowering or ice margin retreat can be interpreted from a plot of the relative positions 634 against exposure ages (Figure 3B). 635

The 'Remove outliers' tool (no. 3) is for diagnosing exposure ages within a dataset 636 derived from a single glacial feature. In an example from a moraine in southern Patagonia 637 (Figure 4A), 14 exposure ages produce a consistent mean and modal age for the feature. 638 However, the spread of ages within the dataset result in a large reduced chi-squared value that 639 is greater than the chi-squared criterion, therefore implying that the mean and standard 640 deviation should not be used to represent the age population (at 95% confidence). Applied to 641 this example, four exposure ages are identified as outliers and are removed from the dataset 642 (Figure 4B). This results in a much tighter cluster of ages and a decreased reduced chi-643 squared that is indicative of a single age population (at 95% confidence). Based on both the 644 645 reduced chi-squared test and gESD outliers test, a weighted mean and standard deviation of

14.22  $\pm$  0.5 ka can be used as the age for this moraine. Ideally, a reason for an outlier should be established whenever one or more are identified – for example, evidence that the sample has experienced surface erosion or post-depositional movement. Outlier removal approaches rely on the assumption that geomorphic processes do not influence each sample equally. If such effects did occur equally – for example, potentially from surface erosion if the samples are of the same lithology and approximately the same age – then the mean ages would shift but the scatter of ages within the dataset would not be significant.



Fig. 3. Exposure ages plotted as A) kernel density estimates for samples from a sequence of moraines
(Ohau II-VI, Lake Ohau, New Zealand; Putnam et al., 2013), and B) a vertical transect recording ice
sheet surface lowering (Mt Suess and Low Ridge, Mackay Glacier, Antarctica; Jones et al., 2015).
These are examples of the plotted outputs from the tools 'Calculate ages' and 'Plot ages', which are
able to highlight temporal and spatial patterns within datasets.



Fig. 4. Exposure ages from a moraine plotted as kernel density estimates A) for the initial raw dataset, 662 and B) following the removal of outliers. The example dataset is from Torres del Paine, southern 663 664 Patagonia (TDPIII, n=14; García et al., 2012). Using the 'Calculate ages' or 'Plot ages' tool, the probability distribution of each sample is plotted in light red and the summed distribution of the 665 666 dataset is plotted as a bold red line. Additionally, the mode (black dashed line), weighted mean (black solid line) and weighted standard deviation (SD; black dotted lines) of the dataset are shown, and the 667 reduced chi-squared ( $\chi_R^2$ ) and associated criterion ( $\kappa$ ) are calculated; if  $\chi_R^2 < \kappa$  then there is a >95 % 668 probability that the data represent a single population (d.f. is degrees of freedom). Four outliers were 669 identified (plotted in grey) and removed in this example using a generalised extreme Studentized 670 deviate (gESD) test with the 'Remove outliers' tool. 671

672

661

673 Two of the iceTEA tools (no. 7 and 8) estimate rates of deglaciation from a transect of674 exposure ages. Average rates of retreat or thinning can be computed using the linear model

675 (no. 7) (Figure 5). This approach is best applied when the position-age relationship of a dataset implies an approximately constant rate of retreat or thinning. In cases where all ages 676 within a transect have overlapping uncertainties, instantaneous retreat or thinning is feasible, 677 but the median and range of rates from the regression analysis provide a more probable 678 estimate based on the age uncertainties (Figure 5D). Transects of exposure ages that imply a 679 variable rate (e.g. periods of both gradual and rapid retreat/thinning) are less suited to this 680 tool, and should instead be used with the Fourier or spline based models (tool no. 8) to 681 compute continuous rates. In Figure 6, modelled surface lowering profiles are plotted for a 682 vertical transect, as well as the corresponding rates of thinning for the period covered by the 683 dataset, for both model approaches. The quality of the fit may vary between approaches, 684 dependent on dataset. In this example, the Fourier Series analysis (number of terms = 3) 685 indicates that the minimum rate of ice surface lowering was equal to or less than 0 cm vr<sup>-1</sup> at 686 multiple times, with a maximum median lowering rate of 14.7 cm  $yr^{-1}$  at 7.3 ka. Using the 687 spline-based approach provides an improved fit, indicating that ice surface lowering was 688 slowest at 10.7 ka, but then accelerated to a maximum median rate of 15.1 cm yr<sup>-1</sup> at 8.1 ka 689 before becoming more gradual after ~6 ka. Irrespective of the approach used to estimate 690 deglaciation rates, the effects from potential outliers within a dataset should be investigated. 691



Fig. 5. Example outputs from estimating average deglaciation rates using the linear model. A) The 694 695 individual linear regressions (grey lines) and the 95% confidence bounds (dashed black lines) are 696 shown for a Monte Carlo (MC) least-squares (LS) linear regression analysis on a horizontal transect 697 of exposure ages. The example data is from the 'Sweden' transect of Cuzzone et al. (2016) and references therein (using the weighted mean ages from individual sites). B) A histogram showing the 698 699 corresponding distribution of retreat rates produced by each iteration of the linear regression analysis. C) and D) are the same as A and B, but for a vertical transect of exposure ages from Mackay Glacier, 700 701 Antarctica (Jones et al., 2015).



Fig. 6. Example output from estimating continuous deglaciation rates using the A) Fourier and B)
spline models. The upper panel is the modelled profile derived from Bayesian penalised spline
regression for an example vertical transect (Scott and Reedy Glaciers, Antarctica; Spector et al.,
2017). The mean exposure ages are also plotted with rectangles representing the age and elevation
uncertainties. The lower panel is the corresponding rate of change. Maximum and minimum rates, and
their respective timings, are also computed.

710

Two iceTEA tools (no. 5 and 6) perform age corrections for a dataset. The 'Correct for 711 surface cover' tool (no. 5) can be used for testing the sensitivity of an exposure age dataset if 712 past cover of rock surfaces is suspected. Figure 7 highlights that the shielding provided by 713 surface cover causes the resulting exposure ages to become older. This effect is greater for a 714 higher density cover material, such as till relative to snow, and for thicker cover, for example 715 50 cm relative to 20 cm (Figure 7). While this approach is useful for examining the effects of 716 shielding by surface cover, the true exposure ages will always be uncertain unless the cover 717 depth and density are confidently known for the full exposure history. 718

The 'Correct for elevation change' tool (no. 6) can be used to understand the potential
exposure age effects from either a long-term approximately constant rate of tectonic rock
uplift/subsidence or GIA changes over the last glacial-interglacial cycle. Tectonic impacts

722 will unsurprisingly be largest at sites near to a plate boundary, such as in the Himalaya. Effects from GIA are both spatially and temporally variable (Jones et al., in review). Broadly, 723 corrected exposure ages will become older if they are derived from a region of significant 724 725 deglaciation (e.g. Norway in Figure 8) due to glacial isostatic depression at the time of initial exposure, can become younger if located at an isostatically elevated, subsiding 'peripheral 726 bulge' region beyond an ice sheet margin (e.g. north-eastern USA in Figure 8), or could be 727 relatively unchanged if they are from a region of negligible surface elevation change (e.g. 728 729 England in Figure 8). The period during which samples have been exposed will also have an effect – for example, a sample that becomes exposed early in the deglaciation (e.g. at 20 ka) 730 will have potentially experienced greater isostatic elevation change than samples initially 731 732 exposed in the Holocene. While applying these corrections should provide more accurate exposure ages – particularly for regions with large elevation changes – these ages are 733 dependent on the GIA model, including uncertainties associated with both the quantification 734 of ice sheet change and Earth rheology, or linear estimate of elevation change. At any 735 particular location, the reliability of the correction also depends on the degree of past 736 atmospheric pressure change in that region (Staiger et al., 2007). This tool will be improved 737 in the future as these effects are better understood and quantified. 738

739



741 Fig. 7. Effects on exposure ages from example scenarios of material covering sampled rock surfaces. 742 The raw, uncorrected exposure ages are shown as kernel density estimates in light red with the summed density estimates of the dataset as a dark red line. The green curves represent the summed 743 density estimates for varying degrees of shielding by overlying materials (individual age distributions 744 745 are not shown for clarity), calculated using the 'Correct for surface cover' tool. The dot-dashed curve is cover by 50 cm of snow (assumed density of 0.27 g cm<sup>-3</sup>), the dashed curve is cover by 20 cm of till 746 (assumed density of 1.8 g cm<sup>-3</sup>), and dotted curve is cover by 50 cm of till. The greater the thickness 747 and density of cover material, the larger the age correction. 748



751 Fig. 8. Effects from GIA. A) The elevation of a sample site relative to present since first exposed, and B) the corresponding change in the site-specific production rate through time. The dashed line 752 assumes no change in GIA, while the solid line is corrected for GIA effects. The orange site is in a 753 region of substantial glacial isostatic uplift (central Norway), the green site was previously 754 isostatically elevated at a 'peripheral bulge' (north-eastern USA), and the purple site is from a region 755 756 of minor past surface elevation change (central England). The examples were generated using the ICE-6G ice model and LSD nuclide scaling model. The high-frequency production rate variability 757 during the last  $\sim 12$  ka is from changes in the solar output; the scaling model uses an average value 758 prior to this time as any variability is undefined (Lifton et al., 2014). 759

#### 761 **4.** Conclusions

iceTEA is an online and MATLAB<sup>©</sup> based suite of tools for plotting and analysing 762 cosmogenic-nuclide surface-exposure data from former glacier and ice sheet margins. The 763 tools allow complex exposure histories to be evaluated using a two-isotope diagram, patterns 764 within exposure age datasets to be identified from kernel density estimate and transect plots, 765 the reliability of exposure ages to be examined with reduced chi-squared and outlier removal 766 tests, linear and continuous rates of retreat or thinning to be estimated, and effects from cover 767 of rock surfaces and time-varying changes in relative elevation to be investigated and 768 corrected ages to be calculated. This paper is not intended to be prescriptive in the 769 approach(es) taken to analysing exposure ages. Our aim is that these tools will allow workers 770 to explore the spatial and temporal patterns in their data in a consistent and inter-comparable 771 way, and also to initiate discussion of further improvements in the application and analysis of 772 773 surface-exposure data.

There is also potential for future iceTEA development. Currently these tools can only be used for <sup>10</sup>Be and <sup>26</sup>Al concentrations and exposure ages, but we intend to expand the code so that it can be used with <sup>3</sup>He, <sup>14</sup>C, <sup>21</sup>Ne and <sup>36</sup>Cl data. The age calculation framework will also be updated following any important revisions of the existing geomagnetic databases, production rates and scaling models. It is also hoped that production rates which have been corrected for both time-varying relative elevation and atmospheric pressure changes will be included in the future. We welcome suggestions for additional plotting or analysis tools.

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#### 784 Appendix 1. Required sample input data

There are two forms of input data required, which can be in a Microsoft<sup>©</sup> Excel<sup>©</sup> (.xlsx) 785 or comma-separated values (.csv) spreadsheet, or in a tab-delimited text file (.txt) without 786 column headings. The standard type of input data is used for all plotting and analysis tools 787 apart from 'Plot two-isotope concentrations', with 15 required columns plus an optional 7 788 columns (22 in total) for importing previously calculated exposure ages. For the 'Plot two-789 isotope concentrations' tool, 17 columns of sample data are required. Templates called 790 'input\_data\_template.xlsx' and 'input\_data\_template\_complex.xlsx' for the two input types, 791 respectively, can be found in the supplementary data, within the compiled MATLAB<sup>©</sup> code 792 and on the iceTEA website. Templates for example datasets are also available. It is possible 793 with the 'Plot two-isotope concentrations' tool to sort and plot bedrock core data where some 794 sections may have been combined for nuclide measurement. In such cases, data should be 795 796 entered with each row representing a separate nuclide measurement (see

797 'GISP2\_input\_complex.xlsx').

798

799 Appendix 2. Overview of the iceTEA online interface.

The home page of iceTEA features links to each of the individual tool interfaces (Figure 800 A1), while a 'Documentation' page provides information on iceTEA, including the 801 MATLAB<sup>©</sup> code and descriptions of the necessary input data formats. On selecting the 802 desired tool, the user will be taken to an interface (e.g. Figure A2). This will include a series 803 804 of stages specific to each tool (Table 1), including Data, Results, Plot Settings and Plot Results. The user can advance through the stages by selecting 'Next', and will be warned if 805 necessary information is missing. In the initial data input stage, sample data in a correctly 806 807 formatted input file (Appendix A1) should be uploaded and the tool parameters should be

- specified. Any results (e.g. calculated ages, corrections, retreat/thinning rate estimates) will
- 809 be displayed in the Results stage. Plots will be shown in the final stage, which can be
- 810 downloaded as both raster-based .png and vector-based .eps files.
- 811



Fig. A1. Home page of iceTEA, which features links to each of the tool interfaces.

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- Fig. A2. An example tool interface. The user can progress through each of the stages (e.g. Data to
- 817 Results to Plot Settings to Plot Results), using the 'Next' button.

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828

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CER

## Highlights

- iceTEA (Tools for Exposure Ages; <u>www.ice-tea.org</u>) is a suite of 8 numerical tools.
- Data can be plotted on a 2-isotope diagram, as density estimates and as a transect.
- Exposure ages can be examined with reduced chi-squared and outlier removal tests.
- Exposure ages can be corrected for surface cover and relative elevation change.
- Rates of ice retreat/thinning can be estimated from linear and spline regression,