ShellChron 0.2.8: A new tool for constructing chronologies in accretionary carbonate archives
from stable oxygen isotope profiles

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Abstract

This work presents ShellChron, a new model for generating accurate age-depth models for high-resolution paleoclimate archives, such as corals, mollusk shells and speleothems. Reliable sub-annual age models form the backbone of high-resolution paleoclimate studies. In absence of independent sub-annual growth markers in many of these archives, the most reliable method for determining the age of samples is through age modelling based on stable oxygen isotope or other seasonally controlled proxy records. ShellChron expands on previous solutions to the age model problem by modelling seasonal variability in the proxy record using a combination of growth rate and temperature sinusoids in sliding window approach. This new approach creates smoother, more precise age-depth relationships for multi-annual proxy records with the added benefit of allowing assessment of the uncertainty on the modelled age. The modular script of ShellChron allows the model to be tailored to specific archives, without being limited to δ18Oc proxy records or carbonate archives, with high flexibility in assigning the relationship between the input proxy and the seasonal cycle. The performance of ShellChron in terms of accuracy and computation time is tested on a set of virtual seasonality records and real coral, bivalve and speleothem archives. The result shows that several key improvements in comparison to previous age model routines enhance the accuracy of ShellChron on multi-annual records while limiting its processing time. The current full working version of ShellChron enables the user to model the age of a 10-year long
1. Introduction

Fast growing carbonate archives, such as coral skeletons, mollusk shells and speleothems, contain a wealth of information about past and present climate and environment (e.g. Urban et al., 2000; Wang et al., 2001; Steuber et al., 2005; Butler et al., 2013). Recent advances in analytical techniques have improved our capability to extract this information and obtain records of the conditions under which these carbonates precipitated at high time resolutions, often beyond the annual scale (Treble et al., 2007; Saenger et al., 2017; Vansteenberge et al., 2019; de Winter et al., 2020a). Key to the interpretation of such records is the development of reliable chemical or physical proxies for climate and environmental conditions which can be measured on a sufficiently fine scale to allow variability to be reconstructed at the desired time resolution. Examples of suitable proxies include observations of variability in carbonate fabric and microstructure and in (trace) elemental and isotopic composition (Frisia et al., 2000; Lough, 2010; Ullmann et al., 2010; Schöne et al., 2011; Ullmann et al., 2013; Van Ramplebergh et al., 2014; de Winter et al., 2017). The unique preservation potential of carbonates in comparison with archives of climate variability at similar time resolutions, such as tree ring records and ice cores, now allows us to recover information about climate and environment of the geological past from these proxies on the (sub-)seasonal scale (Ivany and Runnegar, 2010; Ullmann and Korte, 2015; Vansteenberge et al., 2016; de Winter et al., 2018; 2020b; c; Mohr et al., 2020). The importance of this development cannot be overstated because variability at high (daily and seasonal) resolution constitutes the most significant component of climate variability (Mitchell, 1976; Huybers and Curry, 2006; Zhu et al., 2019). Accurate reconstructions of this type of variability are therefore fundamental to our understanding of Earth’s climate system and critical for projecting of its behavior in the future under greenhouse warming conditions (IPCC, 2018).
A reliable age model is crucial to the interpretation of high-resolution carbonate records. An age model is defined as a set of rules or markers that allows the translation of the location of a measurement or observation on the archive to the time by which the carbonate was precipitated. This translation is required for aligning records from multiple proxies or archives to a common time axis. Age alignment enables data to be intercomparable and to be interpreted in the context of processes playing a role at similar timescales. Age models are based on knowledge about the growth or accretion rate of the archive through time. Many high-resolution carbonate archives contain growth markers on which age models can be based (e.g. Jones, 1983; Le Tissier et al., 1994; Verheyden et al., 2006). These are especially valuable in some mollusk species, in which growth lines demarcate annual, daily, or even tidal cycles (e.g. *Arctica islandica*, Schöne et al., 2005; *Pecten maximus*, Chavaud et al., 2005 and *Cerastoderma edule*, Mahé et al., 2010). However, in many mollusk species and most carbonate archives, such independent growth indicators are absent or too infrequent to (relatively) date high-resolution measurements (Judd et al., 2018; Huyghe et al., 2019). In such cases, age models need to be based on alternative indicators.

The oxygen isotope composition of carbonates ($\delta^{18}$O$_c$) is closely dependent on the isotopic composition of the fluid ($\delta^{18}$O$_w$) and the temperature by which the carbonate is precipitated (Urey, 1948; McCrea, 1950; Epstein et al., 1953). In most natural surface environments, either one or both factors is strongly dependent on the seasonal cycle, one being dominant over the other. This causes carbonates precipitated in these environments to display strong quasi-sinusoidal variations in $\delta^{18}$O$_c$ that follow the seasonal cycle (e.g. Dunbar and Wellington, 1981; Jones and Quitmyer, 1996; Baldini et al., 2008). Examples of this behavior include seasonal cyclicity in sea surface temperatures recorded in the $\delta^{18}$O$_c$ of corals and mollusks and seasonal cyclicity in the $\delta^{18}$O$_w$ of precipitation recorded in speleothems (Dunbar and Wellington, 1981; Schöne et al., 2005; Van Rampaerbergh et al., 2014). These properties make $\delta^{18}$O$_c$ one of the most highly sought-after proxies for climate variability, and high-resolution $\delta^{18}$O$_c$ records are abundant in the paleoclimate literature (e.g. Lachniet, 2009; Lough, 2010; Schöne and Gillikin, 2013 and references therein).

The close relationship between $\delta^{18}$O$_c$ records and the seasonal cycle can also be exploited to estimate variability in growth rate of the archive. This property of $\delta^{18}$O$_c$ curves has been recognized by previous authors, and attempts have been made to quantify intra-annual growth rates from the shape of $\delta^{18}$O$_c$ profiles (Wilkinson and Ivany, 2002; Goodwin et al., 2003; De Ridder et al., 2006; Goodwin et al., 2009;
De Brauwere et al., 2009; Müller et al., 2015; Judd et al., 2018. Over time, these so called “growth models” have improved from fitting of sinusoids to δ¹⁸O c data (Wilkinson and Ivany, 2002; De Ridder et al., 2006) to including increasingly complicated (inter)annual growth rate curves to the model to fit the shape of the δ¹⁸O c data (Goodwin et al., 2003; 2009; Müller et al., 2015; Judd et al., 2018). These later models manage to fit the shape of δ¹⁸O c records well, but they often rely on detailed *a priori* knowledge of growth rate or temperature patterns (e.g. Goodwin et al., 2003; 2009), which causes them to rely on measurements of one or more parameters in the environment. These measurements are not available in studies on carbonate archives from the archeological or geological past. In contrast, the latest model by Judd et al. (2018) is based only on the assumption that growth and temperature follow quasi-sinusoidal patterns and can therefore work with δ¹⁸O c data alone, making it more widely applicable. The simplified parameterization of temperature and growth rate seasonality by Judd et al. (2018) using two (skewed) sinusoids is demonstrated to approximate natural circumstances very well.

However, the approach by Judd et al. (2018) is still limited in its use, because it requires whole, individual growth years to be analyzed separately, resulting in a discontinuous time series when applied on records containing multiple years of δ¹⁸O c data and no solution for incomplete years. In addition, the model has no option to supply information about the less dominant factor that drives δ¹⁸O c values (δ¹⁸O w of sea water in the case of mollusks and corals). Furthermore, only estimates from aragonite records are supported, while the other dominant carbonate mineral, calcite, has a different temperature relationship (Kim and O’Neil, 1997). Finally, neither of the models highlighted above except for the MoGroFun model by Goodwin et al. (2009) include any assessment of the uncertainty of the constructed age model.

Here, a new model for estimating ages of samples in seasonal δ¹⁸O c curves is presented which combines the advantages of previous models while attempting to negate their disadvantages. ShellChron combines a skewed growth rate sinusoid with a sinusoidal temperature curve to model δ¹⁸O c using the SCEUA optimization algorithm (Duan et al., 1992; following Judd et al., 2018). It applies this optimization using a sliding window through the dataset (as in Wilkinson and Ivany, 2002) and includes the option to use a Monte Carlo simulation approach to combine uncertainties on the input (δ¹⁸O c and depth measurements) and the model routine (as in Goodwin et al., 2009). As a result, ShellChron produces a continuous time series with a confidence envelope, supports records from multiple carbonate minerals and allows the user to provide information on the less dominant variable influencing δ¹⁸O c (e.g. δ¹⁸O w) if available. The modular design of ShellChron’s functional script allows parts of the model to be...
adapted and interchanged, supporting a wide range of climate and environmental archives. As a result, the initial design of ShellChron for reconstructing age models in temperature-dominated $\delta^{18}$O$_c$ records from marine bio-archives (e.g. corals and mollusks) presented here can be easily modified for application on other types of records. The routine is worked out into a ready-to-use package for the open-source computational programming language R and is directly available without restrictions, allowing all interested parties to freely modify and build on the base structure to adapt it to their needs (R Core Team, 2020; full package code and documentation in SI1, see also Code availability).

2. Stable oxygen isotope profiles in carbonate archives: The scientific basis

The relationship between $\delta^{18}$O$_c$ and the temperature of carbonate precipitation was first established by Urey (1951) and later refined with additional measurements and theoretical models (Epstein et al., 1953; Tarutani et al., 1969; Grossman and Ku, 1986; Kim and O’Neil, 1997; Coplen, 2007; Watkins et al., 2014; Daëron et al., 2019). Empirical transfer functions for aragonite and calcite by Grossmann and Ku (1986; modified by Dettmann et al., 1999; equation 1) and Kim and O’Neil (1997; equation 2, with VSMOW to VPDB scale conversion following Brand et al., 2014; equation 3) have so far found most frequent use in modern paleoclimate studies, and are therefore applied as default relationships in the ShellChron model (see d18O_model function).

\[
T[°C] = 20.6 - 4.34 \times (\delta^{18}O_c[#VPDB] - \delta^{18}O_w[#VSMOW] + 0.2) (1) 
\]

\[
1000 \times \ln(\alpha) = 18.03 \times \frac{10^3}{(T[°C] + 273.15)} - 32.42
\]

with \( \alpha = \frac{(\delta^{18}O_c[#VPDB] + 1)}{(\delta^{18}O_w[#VPDB] + 1)} \) (2)

\[
\delta^{18}O_w[#VPDB] = 0.97002 \times \delta^{18}O_w[#VSMOW] - 29.98 (3)
\]

To apply these formulae, it is assumed that carbonate is precipitated in equilibrium with the precipitation fluid. The question which carbonates are precipitated in equilibrium has long been subject to debate, and the development of new techniques for measuring the carbonate-water system (e.g. clumped and dual-clumped isotope analyses; Daëron et al., 2019; Bajnai et al., 2020) has led recent authors to...
challenge the assumption that equilibrium fractionation is the norm. These recent findings suggest that kinetic effects in fast-growing carbonate archives or elevated pH in the calcification fluids of some calcifiers (e.g. foraminifera and corals; Rollion-Bard et al., 2003; Zeebe, 2007) force precipitation out of equilibrium, and that true equilibrium is only reached in very slow-growing inorganic carbonates (e.g. Devils Hole vein calcite and subaqueous and cryogenic cave deposits; Coplen, 2007; Bajnai et al., 2020). On the other hand, disequilibrium fractionation likely affected the samples on which empirical transfer functions (equations 1 and 2) were based in a similar way as the samples on which they are applied, potentially eliminating the offset caused by disequilibrium fractionation (Daëron et al., 2019). In addition, the carbonic anhydrase enzyme present in many calcifiers accelerates CO$_2$ hydration at the calcification site, potentially eliminating kinetic effects in carbonate bio-archives whose growth rate would otherwise cause disequilibrium (Uchikawa and Zeebe, 2012). These findings are corroborated by many studies of modern marine calcifiers such as mollusks and corals in which δ$_{18}^{\text{O}}$-based temperatures closely match in situ water temperatures (Dunbar and Wellington, 1981; Jones and Quitmyer, 1996; Ullmann et al., 2010; de Winter et al., 2020c). Therefore, it is widely assumed that many marine calcifiers precipitate their carbonates near isotopic equilibrium and that the empirical transfer functions yield accurate temperature reconstructions. Note that the modular character of ShellChron allows the empirical transfer function to be adapted to the δ$_{18}^{\text{O}}$ record or to the user's preference for alternative transfer functions by a small modification of the $d18O_{\text{model}}$ function, and that future versions of the model will include more options for changing the transfer function by default (see Model description).

As the name suggests, the ShellChron model was initially developed for application on δ$_{18}^{\text{O}}$ records from marine calcifiers (e.g. mollusk shells and corals). ShellChron approximates the temperature evolution at which the carbonate is precipitated by a sinusoidal function (see equation 4 and Table 1; temperature_curve function; visualized in Fig S1), a good approximation of seasonal temperature fluctuations in most marine and terrestrial environments (Wilkinson and Ivany, 2002). Variability in δ$_{18}^{\text{O}}_{\text{w}}$ is also comparatively limited in most marine environments (except for regions with sea ice formation), making the model easy to use in these settings (LeGrande and Schmidt, 2006; Rohling, 2013). Nevertheless, ShellChron includes the option to provide a priori knowledge about δ$_{18}^{\text{O}}_{\text{w}}$, ranging from annual average values to detailed seasonal variability, enabling the model to work in environments with
more complex interaction between δ^{18}O_{w} and temperature on the δ^{18}O_{c} record (see equations 1 and 2).

\[ T[^{\circ}C] = T_{av} + \frac{T_{amp}}{2} \sin\left(\frac{2\pi \cdot (t - T_{pha} + \frac{T_{per}}{4})}{T_{per}}\right) \]  

Table 1: Overview of model parameters

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
<th>Unit</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>(T_{av})</td>
<td>Average temperature</td>
<td>°C</td>
<td>Variable, generally between 0°C–30°C</td>
</tr>
<tr>
<td>(T_{amp})</td>
<td>Temperature range (2*amplitude)</td>
<td>°C</td>
<td>Variable, generally &lt;20°C</td>
</tr>
<tr>
<td>(T_{pha})</td>
<td>Phase of temperature sinusoid</td>
<td>d</td>
<td>0–365 days</td>
</tr>
<tr>
<td>(T_{per})</td>
<td>Period of temperature sinusoid</td>
<td>d</td>
<td>365 days by default</td>
</tr>
<tr>
<td>(G_{av})</td>
<td>Average growth rate</td>
<td>mm/d</td>
<td>Variable, generally between 0–100 mm/day</td>
</tr>
<tr>
<td>(G_{amp})</td>
<td>Range of growth rates</td>
<td>mm/d</td>
<td>Variable, generally &lt;200 mm/day</td>
</tr>
<tr>
<td>(G_{pha})</td>
<td>Phase of growth rate sinusoid</td>
<td>d</td>
<td>0–365 days</td>
</tr>
<tr>
<td>(G_{per})</td>
<td>Period of growth rate sinusoid</td>
<td>d</td>
<td>365 days by default</td>
</tr>
<tr>
<td>(G_{skw})</td>
<td>Skewness factor of GR sinusoid</td>
<td>-</td>
<td>0–100, with 50 meaning no skew</td>
</tr>
<tr>
<td>(D)</td>
<td>Depth along the record</td>
<td>mm</td>
<td>Depends on archive</td>
</tr>
<tr>
<td>(t)</td>
<td>Age</td>
<td>d</td>
<td>Depends on archive</td>
</tr>
<tr>
<td>(L_{win})</td>
<td>Length of sampling window</td>
<td>#</td>
<td>Depends on sampling resolution</td>
</tr>
<tr>
<td>(w)</td>
<td>Weighing factor on sample</td>
<td>-</td>
<td>0–1</td>
</tr>
<tr>
<td>(i)</td>
<td>Position relative to model window</td>
<td>-</td>
<td>0–L_{i}</td>
</tr>
<tr>
<td>(a)</td>
<td>Intercept of sinusoid ((T_{av}) or (G_{av}))</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(A)</td>
<td>Amplitude of sinusoid ((\frac{T_{amp}}{2}) or (\frac{G_{amp}}{2}))</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(P)</td>
<td>Period of sinusoid ((T_{per}) or (G_{per}))</td>
<td>d</td>
<td></td>
</tr>
<tr>
<td>(\phi)</td>
<td>Phase of sinusoid ((T_{pha}) or (G_{pha}))</td>
<td>d</td>
<td></td>
</tr>
</tbody>
</table>

If marine δ^{18}O_{c} records represent one extreme on the spectrum of temperature versus δ^{18}O_{w} influence on the δ^{18}O_{c} record, cave environments, in which δ^{18}O_{c} variability is predominantly driven by δ^{18}O_{w} variability in the precipitation fluid, represent the other extreme (Van Rampelbergh et al., 2014). In its current form, ShellChron takes δ^{18}O_{w} as a user-supplied parameter to model temperature and growth rate variability, but future versions will allow temperature to be fixed, while δ^{18}O_{w} becomes the modelled variable. ShellChron's modular character makes it possible to implement this update without changing the structure of the model. Application of ShellChron on δ^{18}O_{c} records from cave deposits will have to be treated with caution, since drip water δ^{18}O_{w} seasonality (if present) cannot always be approximated by a sinusoidal function and equilibrium fractionation in cave deposits is less common than in bio-archives (Baldini et al., 2008; Daëron et al., 2011; Van Rampelbergh et al., 2014).
Besides temperature (or $\delta^{18}O$) seasonality, ShellChron models the growth rate of the archive to approximate the $\delta^{18}O_c$ record (see equation 5 and Table 1: *growth_rate_curve* function; visualized in Fig S2). Since the growth rate of many carbonate archives varies seasonally, a quasi-sinusoidal model for growth rate seems plausible (e.g. Le Tissier et al., 1994; Baldini et al., 2008; Judd et al., 2018). However, as discussed in Judd et al. (2018), the occurrence of growth cessations (growth rate = 0) and skewness in seasonal growth patterns calls for a more complex growth rate model that can take these properties into account. Therefore, ShellChron uses a slightly modified version of the skewed sinusoidal growth function described by Judd et al. (2018; equation 5). Note that the added complexity of this function does not preclude the modelling of growth rate functions described by a simple sinusoid (no skewness; $G_{skw} = 50$) or even constant growth through the year ($G_{amp} = 0$; see Table 1).

$$G\ [mm/yr] = G_{av} + \frac{G_{amp}}{2} \sin \left( \frac{2\pi \times (t[d] - G_{pha} + G_{per} \times S)}{p} \right)$$

with \( S = \begin{cases} 100 - G_{skw} \ , & \text{if } t[d] - G_{pha} < G_{per} \\ \frac{G_{skw}}{50} \ , & \text{if } t[d] - G_{pha} \geq G_{per} \end{cases} \) (5)

Contrary to previous $\delta^{18}O_c$ growth models, ShellChron allows uncertainties on the input variables (depth and $\delta^{18}O_c$ measurements) as well as uncertainties of the full modelling approach to be propagated, providing confidence envelopes around the chronology. Uncertainty propagation is optional and can be skipped without compromising model accuracy. Standard deviations of uncertainties on input variables (depth and $\delta^{18}O_c$) can be provided by the user, while model uncertainties are calculated from the variability in model results of the same datapoint obtained from overlapping simulation windows (see *growth_model* function). Measurement errors are combined by projecting Monte Carlo simulated values for depth and $\delta^{18}O_c$ measurements on the modelled $\delta^{18}O_c$ curve through an orthogonal projection (equation 6: *mc_err_orth* function; visualized in Fig S3). The measurement uncertainty projected on the depth domain is then combined with the model uncertainty to obtain pooled uncertainties in the depth domain, which are propagated through the modelled $\delta^{18}O_c$ record to obtain uncertainties on the model result in the age domain. As a result of the sliding window approach in ShellChron, model results for datapoints situated at the edges of windows are more sensitive to small changes in the modelled parameters and therefore possess a larger model uncertainty. To prevent these less certain model estimates from affecting the stability of the model, model results were given more weight the closer they
were situated towards the center of the model window (see equation 7 in export_results function; see also Fig. S4). This weighing is also incorporated in uncertainty propagation through a weighted standard deviation (see equation 8 from the sd_wt function).

\[ \sigma_{\text{meas}} = \sqrt{\left( \frac{D_{\text{sim}} - \bar{D}_{\text{sim}}}{\sigma_D} \right)^2 + \left( \frac{\delta^{18}O_{\text{sim}} - \bar{\delta^{18}O}_{\text{sim}}}{\sigma_{\delta^{18}O}} \right)^2} \] (6)

\[ w[i] = 1 - \frac{2i}{L_{\text{window}} - 1} \] (7)

\[ \sigma_{\text{weighted},i} = \sqrt{\frac{w_i \times (x_i - \bar{x})^2}{\sum w[i] \times \frac{N - 1}{N}}} \] (8)

3. Model description

ShellChron is organized in a series of functions that describe the step-by-step modelling process. A schematic overview of the model is given in Fig. 1. A wrapper function (wrap_function) is included which carries out all steps of the model procedure in succession to promote ease of use.
Figure 1: Schematic overview of ShellChron. Names in *italics* refer to functions (encapsulated in rounded rectangular boxes) and operations within functions. Rectangular boxes represent data. Arrows represent the flow of information between model components. Note that some operations are encapsulated in functions (e.g. *Error propagation* in *export results*) and that some functions are only used within other functions (e.g. *peakid* in *cumulative_day*). All data structures outside *wrap_function* represent input and output of the model. Detailed documentation of all functions and operations in ShellChron is provided in SI1.
Data is imported through the `data_import` function, which takes a comma-separated text file (CSV) with the input data. Data files need to contain columns containing depth ($D$) and $\delta^{18}O_c$ data, a column marking years in the record and two optional columns containing uncertainties on depth ($\sigma(D)$, one standard deviation) and $\delta^{18}O_c$ ($\sigma(\delta^{18}O_c)$, one standard deviation) respectively (see example in SI2 and Figure 2).

The function uses the year markers (third column) as guidelines for defining the minimum length of the model windows to ensure that all windows contain at least one year of growth. Consecutive windows are shifted by one datapoint, yielding a total number of windows equal to the sample size minus the length of the last window. The result of the model does not otherwise depend on user-provided year markers, instead basing the age result purely on simulations of the $\delta^{18}O_c$ data.
Figure 2: Schematic overview of the structure of the result array in which ShellChron stores the raw results of each model window. Data is stored in three dimensions: The sample number (rows in the figure), the window number (columns in the figure) and the number of modelled parameters (represented by the stacked table “sheets” in the figure). Note that the first 5 columns of each “sheet” represent the user-provided input data (see example in SI2), and that the model result data starts from column 6. The window length is determined by the user-provided indication of year transitions (column 3). Rows of dots in the figure are placeholders for (input or result) values. Shading of these dots in the window columns indicate differential weighing of modelled values in function of their location relative to the sliding window. The horizontal box shows how these weighing factors within each sample window (in vertical direction) result in weighing of different estimates of modelled parameters for the same data point (in horizontal direction). Shading of input data and window number towards the bottom and right edge of the figure,
respectively, indicates that the number of input values (and thus simulation windows) is only limited to the length of the input table and may therefore continue indefinitely (at the expense of longer computation times, see Figure 5 in Model performance).
The core of the model consists of simulations of overlapping subsamples (windows) of the depth and δ¹⁸Oc data described by the run_model function (see Fig. 1 and 2). Data and window sizes are passed from data_import onto run_model along with user-provided parameters (e.g. δ¹⁸Ow information; see Fig. 1). run_model loops through the data windows and calls the growth_model function, which fits a modelled δ¹⁸Oc vs. depth curve through the data using the SCEUA optimization algorithm (see Duan et al., 1992). The simulated δ¹⁸Oc curve is produced through a combination of a temperature sinusoid (temperature_curve function; see equation 4 and Fig. S1) and a skewed growth rate sinusoid (growth_rate_curve; see equation 5 and Fig. S2), with temperature data converted to δ¹⁸Oc data through the d18O_model function (equation 1). Starting values for the parameters describing temperature and growth rate curves are obtained by estimating the annual period (P) through a spectral density estimation and applying a linearized sinusoidal regression through the δ¹⁸Oc data (sinreg function; see equation 9). In addition, growth_model takes a series of fixed parameters describing the method for SCEUA optimization (see Duan et al., 1992; Judd et al., 2018) and the upper and lower bounds for parameters describing temperature and growth rate curves (see SI3). If uncertainties on depth and δ¹⁸Oc data are provided, growth_model calls the mc_err_orth function to propagate these errors through the model result (see equation 6 and Fig S3).

\[
\delta^{18}O_{\text{VPDB}} = I + \frac{A}{2} \sin \left( \frac{2\pi \cdot (D - \varphi + \frac{P}{4})}{P} \right),
\]

linearized as: \[
\delta^{18}O_{\text{VPDB}} = a + b \sin \left( \frac{2\pi \cdot D}{P} \right) + c \cos \left( \frac{2\pi \cdot D}{P} \right),
\]

with \( I = a; A = \sqrt{b^2 + c^2} \) and \( \varphi = P \left( 0.25 - \frac{\cos^{-1} \left( \frac{b}{A} \right)}{2\pi} \right) \) (9)

The run_model function returns an array listing day of the year (1–365), temperature, δ¹⁸Oc, growth rate and (optionally) their uncertainty standard deviations as propagated from uncertainties on the input data ("result array"; see Fig. 2 and SI4). In addition, a matrix containing the optimized parameters of temperature and growth rate curves is provided, yielding information about the evolution of mean values, phases, amplitudes, and skewness of seasonality in temperature and growth rate along the record ("parameter matrix", see Fig. 1 and SI5). To construct an age model for the entire record, the modelled timing of growth data, expressed as day relative to the 365-day year, needs to be converted into a
cumulative time series listing the number of days relative to the start of the first year represented in the record (rather than relative to the start of the year in which the datapoint is found). This requires year transitions (transitions from day 365 to day 1) to be recognized in all the model results. The `cumulative_day` function achieves this by aggregating information about places where the beginning and end of the year is recorded in individual window simulations and applying a peak identification algorithm (`peakid` function) to find places in the record where year transitions occur (see Supplementary Methods). Results of the timing of growth for each sample (in day of the year) are converted to a cumulative time scale using their positions relative to these recognized year transitions (Supplementary Methods).

In a final step (described by the `export_results` function), the results from overlapping individual modelling windows are combined to obtain mean values and confidence envelopes of the result variables (age, δ¹⁸O, δ¹⁸O-based temperatures and growth rates) for each sample in the input data. If uncertainties on the input variables were provided, these are combined with uncertainties on the modelling result calculated from results of the same datapoint on overlapping data windows by pooling the variance of the uncertainties (equation 10). Throughout this merging of data from overlapping windows, results from datapoints on the edge of windows are given less weight than those from datapoints near the center of a window (see equation 7 and Fig. S4). This weighing procedure corrects for the fact that datapoints near the edge of a window are more susceptible to small changes in the model parameters and are therefore less reliable than results in the center of the window. Finally, summaries of the simulation results and the model parameters including their confidence intervals are exported as comma-separated (CSV) files. In addition, `export_results` supports optional exports of figures displaying the model results and files containing raw data of all individual model windows (equivalent to “sheets” of the result array, see Fig. 2 and SI4).

\[
VAR_{pooled} = \frac{\sum_i((N_i - 1) \cdot VAR_i \cdot w_i)}{\sum_i(N_i) - n}
\]

in which \(w\) = weight of the individual reconstructions, \(N\) is the sample size and \(n\) is the number of reconstructions (indexed by \(i\)) that is combined (10)

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Footnotes:

1. https://doi.org/10.5194/gmd-2020-401
2. Preprint. Discussion started: 12 February 2021
3. © Author(s) 2021. CC BY 4.0 License.
4. Model performance

The performance of ShellChron was tested on two virtual datasets: a δ¹⁸Oc record constructed from a simulated temperature sinusoid with added stochastic noise (Case 1; SI6) and one based on a real high-resolution sea surface temperature and salinity record measured on the coast of Texel island in the tidal basin of the Wadden Sea in the north of the Netherlands (Texel, see details in SI7 and de Winter et al., 2020d and Supplementary Methods). In addition, three modern carbonate δ¹⁸Oc records were internally dated using ShellChron: a tropical stony coral (Porites lutea; hereafter: coral) from the Pandora Reef (Great barrier Reef, NE Australia; Gagan et al., 1993; see SI8), a Pacific oyster shell (Crassostrea gigas; hereafter: oyster) from List Basin in Denmark (Ullmann et al., 2010; see SI8) and a temperate zone speleothem from Han-sur-Lesse cave (Belgium; hereafter: speleothem; see Vansteenberge et al., 2019; see SI8). Finally, ShellChron’s performance in terms of computation time and accuracy is compared to that of the most comprehensive pre-existing δ¹⁸Oc-based age model (by Judd et al., 2018) on simulated temperature sinusoids of various length and sampling resolutions to which stochastic noise was added (sensu Case 1; de Winter et al., 2020d; see SI9). The latter also demonstrates the scalability of ShellChron and its application on a variety of datasets. Timing comparisons were carried out using a modern laptop (Dell XPS13-7390; Dell Inc., Round Rock, TX, USA) with an Intel Core i7 processor (8 MB cache, 4.1 GHz clock speed, 4 cores, Intel Corporation, Santa Clara, CA, USA), 16 GB LPDDR3 RAM and a SSD drive running Windows 10. Note that ShellChron was built and tested successfully on Mac OS, Fedora Linux and Ubuntu Linux as well.
Figure 3: Result of applying ShellChron on the two virtual datasets: **Case 1** (top, see SI6) and **Texel** (bottom, see SI7). Leftmost panels show the model fit of individual sample windows (red) on the data (black, including horizontal and vertical error bars), with in the top left Spearman’s correlation coefficients ($\rho$) and standard deviations on the $\delta^{18}$Oc estimate ($\sigma_{est}$). Right panels show the resulting age model (red, including shaded 95% confidence level) compared with the real age-depth relationship of both records. Histograms in the top left of age-depth plots show the offset between modelled and measured $\delta^{18}$Oc (as visualized in the left panel) with standard deviations of the $\delta^{18}$Oc offset ($\sigma_{off}$) and offset averages ($\mu$). Histograms in the bottom right of age-depth plots show the offset between modelled and actual ages (in days) of each datapoint, including standard deviations on the age accuracy ($\sigma_{acc}$) and mean age offset ($\mu$). Note that the last 2 years’ worth of data in the **Texel** dataset (shaded in yellow) show a positive offset of almost 1 year due to an aberration in the data around 60 mm (see discussion in text).
Results of running ShellChron on Case 1 and Texel datasets (Fig. 3) show that modelled $\delta^{18}$O$_c$ records in individual windows closely match the data. A summary of ShellChron performance statistics is given in Table 2. In both virtual datasets, $\delta^{18}$O$_c$ estimates are equally distributed above and below the $\delta^{18}$O$_c$ data ($\overline{\Delta^{18}O_c} = 0.0$‰; Spearman’s $\rho$ of 0.79 and 0.71 for Case 1 and Texel datasets respectively) and show no seasonal bias (see SI10) in both datasets. The fact that this is also the case for the Texel dataset, which is skewed towards growth in the winter season and includes relatively strong seasonal variability in $\delta^{18}$O$_w$, shows that ShellChron is not sensitive to such subtle (though common) variability in growth rate or $\delta^{18}$O$_w$. In general, ShellChron’s mean age assignment is accurate on a monthly scale (age offsets of -19 ± 39 d and +31 ± 128 d for Case 1 and Texel datasets respectively). The Texel data contains some notable exceptions near the end of the record, where the sampling resolution is reduced (see SI7) resulting in an overestimation of the age for data in the last two years in the record. On closer inspection, the inaccuracies result from a persistent reduction of $\delta^{18}$O$_c$ in the winter season around 60 mm along the record which is interpreted by the model as an extra annual cycle. This glitch results from the interplay of seasonally low $\delta^{18}$O$_w$ values and stochastic noise in high-resolution records and warrants a posteriori inspection of model results by the user. The offset in the last part of the record can be easily spotted by inspecting the growth curve and amended by subtracting the extra year from the affected datapoints. After correction, the accuracy of modelling the Texel age becomes (-22 ± 80 d).
Table 2: Overview of datasets and model results

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Resolution</th>
<th>Length</th>
<th>δ¹⁸Oc seasonal range</th>
<th>Complications</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>50 yr⁻¹</td>
<td>6 yr</td>
<td>~4.3‰</td>
<td>None</td>
</tr>
<tr>
<td>Texel</td>
<td>26–45 yr⁻¹</td>
<td>10 yr</td>
<td>~4‰</td>
<td>Variable δ¹⁸Oc, Variable GR</td>
</tr>
<tr>
<td>Coral</td>
<td>30–49 yr⁻¹</td>
<td>6 yr</td>
<td>~1.7‰</td>
<td>Variable GR</td>
</tr>
<tr>
<td>Oyster</td>
<td>23–45 yr⁻¹</td>
<td>3.5 yr</td>
<td>~3‰</td>
<td>Variable δ¹⁸Oc, Variable GR</td>
</tr>
<tr>
<td>Speleothem</td>
<td>4–13 yr⁻¹</td>
<td>14 yr</td>
<td>~0.5‰</td>
<td>Variable δ¹⁸Oc, Variable GR, Non-sinusoidal δ¹⁸Oc-forcing</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Dataset</th>
<th>δ¹⁸Oc offset</th>
<th>Age offset</th>
<th>Spearman’s p</th>
<th>Observations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>0.0 ± 0.91‰</td>
<td>-19 ± 39 d</td>
<td>0.79</td>
<td></td>
</tr>
<tr>
<td>Texel</td>
<td>0.0 ± 0.77‰</td>
<td>+31 ± 128 d</td>
<td>0.71</td>
<td>Last 2 years off</td>
</tr>
<tr>
<td>Coral</td>
<td>0.0 ± 0.15‰</td>
<td>-22 ± 44 d</td>
<td>0.96</td>
<td></td>
</tr>
<tr>
<td>Oyster</td>
<td>0.0 ± 0.35‰</td>
<td>-9 ± 53 d</td>
<td>0.91</td>
<td>Reduced accuracy near growth stops</td>
</tr>
<tr>
<td>Speleothem</td>
<td>0.0 ± 0.13‰</td>
<td>105 ± 166 d</td>
<td>0.71</td>
<td>Only reliable on inter-annual scale</td>
</tr>
</tbody>
</table>
Figure 4: Overview of model results for the three test datasets from real carbonate archives: (A) coral, (B) oyster and (C) speleothem. Lower panels indicate the fit of individual model windows (in red) with the data (in black) while upper panels show the age model (in red) compared to the “true” age-depth relationship with histograms showing model accuracy (in days, top left) and model fit ($\delta^{18}O$ offset in ‰, bottom right). Color scheme follows Figure 3. Note that the true age-depth relationship is not known for these natural records, but is estimated using known growth seasonality (coral), comparison with in situ temperature and salinity measurements (oyster) or simply by interpolating between annual growth lines (speleothem). See Supplementary Methods for details.
Results of modelling natural carbonate records (Fig. 4 and Table 2) illustrate the effectiveness of ShellChron on different types of records. Performance clearly depends on the resolution of the record and the regularity of seasonal variability contained within. As in the virtual datasets, modelled δ\(^{18}\)O\(_{c}\) successfully mimic δ\(^{18}\)O\(_{c}\) data in all records (\(\Delta^{18}\)O\(_{c}\) = 0.0; Spearman’s \(p\) of 0.96, 0.91 and 0.71 for coral, oyster and speleothem respectively). No consistent seasonal bias is observed in \(\Delta^{18}\)O\(_{c}\) and model accuracy (\(p>0.05\); see Table 2 and SI10), despite significant (seasonal and inter-annual) variability contained in the records (especially in oyster and speleothem records). When comparing the accuracy of these records, it must be noted that the “real” age of the samples in these natural carbonates is not known with accuracy. Model results are instead compared with age models constructed using conventional techniques such as matching δ\(^{18}\)O\(_{c}\) profiles with local temperature and/or δ\(^{18}\)O\(_{w}\) variability (oyster and coral records) or even merely by linear interpolation between annual markers in the record (speleothem record; see Supplementary Methods). Despite this caveat, testing results clearly show that the least complicated record (coral; Fig. 4a), characterized by minimal variability in δ\(^{18}\)O\(_{w}\) and growth rate and a high sampling density, has the best overall model result (\(\Delta^{18}\)O\(_{c}\) = 0.0 ± 0.15 compared to a ~1.7‰ seasonal range; \(p = 0.96; \Delta t = -22 \pm 44\) d; see Table 2). The oyster record (Fig. 4b), which has strong seasonal variability in growth rate and δ\(^{18}\)O\(_{w}\) also yields a very reliable age model (\(\Delta^{18}\)O\(_{c}\) = 0.0 ± 0.15 compared to a ~3‰ seasonal range; \(p = 0.91; \Delta t = -9 \pm 53\) d; see Table 2). The speleothem record (Fig. 4c), plagued by lower sampling resolution, large inter-annual δ\(^{18}\)O\(_{c}\) variability, restricted δ\(^{18}\)O\(_{c}\) seasonality and a lack of clearly seasonal δ\(^{18}\)O\(_{c}\) forcing, yields the least reliable model result (\(\Delta^{18}\)O\(_{c}\) = 0.0 ± 0.13 compared to a ~0.5‰ seasonal range; \(p = 0.71; \Delta t = 105 \pm 166\) d; see Table 2).

Note that the accuracy figure provided for the speleothem record is based on comparison with an age model based on linear interpolation between annual growth lines. Since no reliable information is available on sub-annual variability in growth rates in this record, ShellChron results cannot be validated at the sub-annual scale in this case.
Figure 5: Overview of the result of timing ShellChron and the Judd et al. (2018) model on the same datasets (A), comparing the accuracies of both models (B) and comparing the accuracy as calculated by ShellChron with the real offset in the age model (C). In (A) and (B), low resolution datasets are plotted in blue, while high-resolution datasets plot in red. Solid lines represent ShellChron and dashed lines show performance of the Judd et al. model. The black box in (A) and (B) highlights the dataset used in (C). In (C), grey lines, bars and boxplot indicate true offset of the model from the actual sample age, while red lines, bars and boxplot show the accuracy of the model as calculated from the propagated errors on model and input data.
The performance of both ShellChron and the Judd et al. model in terms of computation time linearly increases with the length of the record (in years; see Fig. 5, Fig. S5 and SI9). Computation time of ShellChron on the high-resolution test dataset (50 samples/yr) increases very steeply with the length of the record in years (~21 minutes per additional year), while the low-resolution dataset (16 samples/yr) shows a slower increase (~5 minutes per additional year; Fig. 5A). This contrasts with the model from Judd et al., which requires only slightly more time on high-resolution data than on low-resolution datasets (~7 and ~10 minutes per additional year, respectively). The difference is explained by the sliding window approach applied in ShellChron, which requires more SCEUA optimization runs per year in high-resolution datasets than in low resolution datasets. When plotted against the number of calculation windows or samples in the dataset, running ShellChron on low-resolution and high-resolution datasets require a similar increase in computation time (~0.4 minutes, or 24 seconds, per additional sample/window; Fig. S5). ShellChron thus outcompetes the Judd et al. model in terms of computation time in datasets with fewer than ~20 samples per year, even though more SCEUA optimizations are required.

The key computational improvement in ShellChron is the application of a sinusoidal regression before each SCEUA optimization to estimate the initial values of the modelled parameters (sinreg function; see equation 9 and Fig. 1 in Model description). Since carbonate archives are rarely sampled for stable isotope measurements above 20 samples per year (e.g. Goodwin et al., 2003; Schöne et al., 2005; Lough, 2010 and references therein), the disadvantage of a steep computational increase for very high-resolution archives is, in practice, a favorable tradeoff for the added control on model and measurement uncertainty and smoother inter-year transitions ShellChron offers in comparison to previous models. The similarity of ShellChron’s accuracy in the low- and high-resolution datasets demonstrates its robustness across datasets with various sampling resolutions (see also Table 2 and Fig. 4B).

Longer computation times in the Judd et al. model result in better accuracy on the modelled age compared to the present version of ShellChron on the scale of individual datapoints (see Fig. 5). However, this advantage is rapidly lost when records containing multiple years are considered (Fig. 5B). The advantage of the ShellChron model is its application of overlapping model windows, which smooth out the transitions between modelled years and eliminate accumulations of model inaccuracies when records grow longer. In addition, contrary to previous models, ShellChron does not rely on user-defined year boundaries, which may introduce mismatches between subsequent years to be propagated.
through the age model, even in ideal datasets such as Case 1 (Fig. 5B; see also Supplementary Methods). By comparison, the overall accuracy of ShellChron is much more stable within and between datasets of different length, while rarely introducing offsets of more than a month. More importantly, where ShellChron takes into account the uncertainty on input parameters, this uncertainty is not considered in most previous models (the MoGroFun model of Goodwin et al., 2003 being the exception). The added uncertainty caused by input error is higher in less regular (sinusoidal) $\delta^{18}O_c$ records and in records with lower sampling resolution, causing the uncertainties on the Judd et al., model reported here for the ideal, high-resolution Case 1 dataset to be over-optimistic. If ShellChron’s model accuracy is insufficient, its modular character allows the user to run the SCEUA algorithm to within more precise optimization criteria by changing the model parameters (see SI3). However, this adaptation comes at a cost of longer computation times.

The estimated uncertainty envelope (95% confidence interval) on the modelled age calculated by the error propagation algorithm in ShellChron (24 ± 14 d) on average slightly underestimates the actual offset between modelled age and real age in the Case 1 record (31 ± 24 d; $p_{\text{difference}} < 0.05$; Fig. 5C). The foremost difference between modelled and real uncertainty on the result is that the modelled uncertainty yields a more smoothed record of uncertainty compared to the record of actual offset of the model (Fig. 5C). ShellChron’s uncertainty calculations are partly based on comparing overlapping model windows, thereby smoothing out short term variations in model offset. The uncertainty of the model result (both real and modelled) shows regular variability with a period of half a year (Fig. 5C). Comparing this variability with the phase of the record (of which 6 years are plotted in Fig. 3A) reveals that the uncertainty of the model is positively correlated to the slope of the $\delta^{18}O_c$ record. This is expected, because in parts of the record with steep $\delta^{18}O_c$-depth slopes, the local age model result is more sensitive to small changes in the depth domain, caused either by uncertainty in the model fit or propagated uncertainty on the depth value defined by the user.

5. Applications and discussion

Its new features compared to previous age model routines make ShellChron a versatile package for creating age models in a range of high-resolution paleoclimate records. The discussion above demonstrates that ShellChron can reconstruct the age of individual $\delta^{18}O_c$ samples within monthly
This level of precision is sufficient for accurate reconstructions of seasonality, defined as the difference between warmest and coldest month (following USGS definitions; O'Donnell and Ignizio, 2012). While an improvement on this uncertainty could be of potential interest for ultra-high-resolution paleoclimate studies (e.g., sub-daily variability; see Sano et al., 2012; Yan et al., 2020; de Winter et al., 2020a), the increase in computation time and the sampling resolution such detailed age models demand render age modelling from δ¹⁸O records inefficient for this purpose. The sampling resolution for high-resolution carbonate δ¹⁸O records in the literature does not typically exceed 0.1 mm due to limitations in sampling acquisition (e.g., micromilling), which even in fast-growing archives limits the resolution of these records to several days at best (see Gagan et al., 1994; Van R JMParlebergh et al., 2014; de Winter et al., 2020c). While in some archives, high-resolution (<100 µm) trace element records could be used to capture variability beyond this limit, the monthly age resolution of ShellChron is sufficient for most typical high-resolution paleoclimate studies.

The ability to produce uninterrupted age models from multi-year records while considering both variability in δ¹⁸Ow and uncertainties on input parameters represent major advantages of ShellChron over previous age modelling solutions. As a result, ShellChron can be applied on a wide range of carbonate archives (see Fig. 4 and Table 2). However, testing ShellChron on different records highlights the limitations of the model inherited through its underlying assumptions. The most accurate model results are obtained on records with minimal growth rate and δ¹⁸Ow variability and a nearly sinusoidal δ¹⁸Oc record, such as tropical coral records (Fig. 4A; Gagan et al., 1994). In records where large seasonal variability in growth rate and δ¹⁸Ow does occur, such as in intertidal oyster shells, ShellChron’s accuracy slightly decreases, especially near growth hiatuses in the record (see Fig. 4B; Ullmann et al., 2010). A worst-case scenario is represented by the speleothem record, which not only suffers from much slower and more unpredictable growth rates but responds to variability in drip water in the cave rather than temperature seasonality, one of the assumptions underlying the current version of ShellChron (Fig. 4C; Vansteenberghe et al., 2019). Despite these problems, ShellChron yields an age model that is remarkably accurate on an annual timescale, which is as good as, or better than, the best age model that can be obtained by applying layer counting on the most clearly laminated parts of the speleothem (e.g., Verheyden et al., 2006). It must be noted that, while this is an encouraging result, a major reason for the model’s success is the fact that the Proserpine speleothem used in this example is known to receive significantly seasonal (though not sinusoidal) drip water volumes and concentrations...
(Van Rampelbergh, 2014). Variability in drip water properties and cave temperatures are known to differ strongly between cave systems, and ShellChron can therefore only be applied with confidence on speleothem records if consistent seasonal variability in these parameters can be demonstrated (Fairchild et al., 2006; Lachniet, 2009).

The difficulty of applying age model routines on speleothem records highlights one of the main advantages of ShellChron over pre-existing age model routines, namely its modular character. Since δ¹⁸O records from some carbonate archives, such as speleothems, cannot be described by the standard combination of temperature and growth rate sinusoids on which ShellChron is based (in its current version), the possibility to adapt the “building block” functions used to approximate these δ¹⁸O records (d₁⁸O_model, temperature_curve and growth_rate_curve; see Fig. 1) while leaving the core structure of ShellChron intact greatly augments the versatility of the model. The freedom to adapt the building blocks used to approximate the δ¹⁸O record theoretically enables ShellChron to model sub-annual age-depth relationships in any record as long as the seasonal variability in the variables used to model the input data are predictable and can be represented by a function. For example, since speleothem δ¹⁸O records often depend on variability in the δ¹⁸Ow value of the drip water, a function describing this variability through the year can replace the temperature_curve function to create more accurate sub-annual age models for speleothems (e.g. Mattey et al., 2008; Lachniet, 2009; Van Rampelbergh et al., 2014). Similarly, the growth_rate_curve function can be modified in case the default skewed sinusoid does not accurately describe the extension rate of the record under study, and the d₁⁸O_model function can be adapted to feature the most fitting δ¹⁸O-temperature or δ¹⁸O-δ¹⁸Ow relationship.

By extension, flexibility in the definition of “building block” functions used to approximate the input data paves the way for future application beyond carbonate δ¹⁸O records. The seasonal variability in δ¹⁸O in some ice cores can be approximated by a stable and unbiased temperature relationship (van Ommen and Morgan, 1997). ShellChron can therefore be modified to date sub-annual samples in these ice core records and reconstruct seasonal variability in the high latitudes through the Quarternary. Similarly, inter-annual δ¹⁸O variability in tree ring records are demonstrated to record variability in precipitation through the year, and this variability can be modelled to improve sub-annual age models in these records (Xu et al., 2016). More generally, the field of dendrochemistry has recently developed additional chemical
proxies for seasonality (e.g. trace element concentrations), which can be measured on smaller sample volumes (and thus greater resolution) to obtain ultra-high-resolution records on which (sub-annual) dating can be based (e.g. Poussart et al., 2006; Superville et al., 2017). A similar development has taken place in the study of carbonate bio-archives such as corals and mollusks, of which some show strong, predictable seasonal variability in trace elements (e.g. Mg/Ca and Sr/Ca ratios) which can be used to accurately date these records (de Villiers et al., 1995; Sosdian et al., 2006; Durham et al., 2017). Minor changes in the “building block” functions using empirical transfer functions for these trace element records will enable ShellChron to capitalize on these relationships and reconstruct sub-annual growth rates with improved precision due to the higher precision with which these proxies can be measured compared to δ¹⁸Oc records. Finally, the application of ShellChron for age model construction is not necessarily limited to the seasonal cycle, as other major cycles in climate (e.g. tidal, diurnal or Milankovitch cycles) leave similar marks on climate records and can thus be used as basis for age modelling (e.g. Sano et al., 2012; Huyghe et al., 2019; de Winter et al., 2020a; Sinnesael et al., 2020). It must be noted that, since ShellChron was developed for modeling based on annual periodicity, applying it on other timescales would require more thorough adaptation of the model code than merely adapting the “building block” functions to support additional proxy systems.

While age reconstructions are the main aim of ShellChron, the model also yields information about the temperature and growth rate parameters used in each simulation window to approximate the local δ¹⁸Oc curve. These parameters hold key information about the response of the archive to seasonal changes in the environment, such as the season of growth, relationships between growth rate and temperature and the temperature range that is recorded. By combining these parameters with records of influential environmental variables such as seawater chlorophyl concentration or local precipitation patterns, much can be learned about the climate archive itself and its response to environmental variables, in addition to the climate or environmental change it records. Study examples include the relationship between growth rate of marine calcifies and phytoplankton abundance or the correlation between precipitation patterns and chemical variability in speleothems. While such discussion is beyond the scope of this work, examples of parameter distributions are provided in SI5, and the application of modelled growth rate parameters in bivalve sclerochronology is discussed in more detail in Judd et al. (2018). Note that the sliding window approach of ShellChron produces records of changing temperature and growth rate
parameters at the scale of individual samples (albeit smoothed by the sliding window approach) rather than annually, as in Judd et al. (2018).

6. Conclusions

ShellChron offers a novel, open-source solution to the problem of dating carbonate archives for high-resolution paleoclimate reconstruction on a sub-annual scale. Based on critical evaluation of previous age models, building on their strengths while attempting to eliminate their weaknesses, ShellChron provides continuous age models based on $\delta^{18}O_c$-profiles in these archives with monthly accuracy, taking into account the uncertainties associated with both the model itself and the input data. The monthly accuracy of the model, as tested on a range of virtual and natural datasets, enables its application for age determination in studies of seasonal climate and environmental variability. Higher accuracies can be reached at the cost of longer computation times by adapting the model parameters, but age determinations far beyond the monthly scale are unlikely to be feasible considering the limitations on sampling resolution and measurement uncertainties on $\delta^{18}O_c$ records. ShellChron’s computation times on datasets with sampling resolutions typical for the paleoclimatology field (up to 20 samples/yr) remain practical and competitive with previous model solutions, despite adding several features that improve the versatility and interpretation of model results. Its modular design allows ShellChron to be adapted to different situations with comparative ease. It thereby functions as a platform for age-depth modelling on a wide range of climate and environmental archives and is not limited in its application to the $\delta^{18}O_c$ proxy, the carbonate substrate or even to the annual cycle, as long as the relationship between the proxy and the extension rate of the archive on a given time scale can be parameterized. Future improvements will capitalize on this variability, expanding ShellChron beyond its current dependency on the $\delta^{18}O_c$-temperature relationship in carbonates. Members of the high-resolution paleoclimate community are invited to contribute to this effort by adapting the model for their purpose.

Code availability

ShellChron is worked out into a fully functioning package for the open-source computational language R (version 3.5.0 or later; R Core Team, 2020). The most recent full version (v0.2.8) of the ShellChron
passed the code review of the Comprehensive R Archive Network (CRAN) and is freely available for
download as an R package on the CRAN server (see https://CRAN.R-project.org/package=ShellChron).
The CRAN server entry also includes detailed line-by-line documentation of the code and working
eamples for every function. In addition, the development version of ShellChron (currently v0.2.9.9000)
is available on GitHub (https://github.com/nielsjdewinter/ShellChron). Those interested in adapting
ShellChron for their research purposes are invited to do so here. Code and documentation, together
with all supplementary files belonging to this study, are also available on the open-source online

Author contribution

NJV designed the study, wrote the model script, carried out the test calculations and wrote the
manuscript.

Competing interests

There were no competing interests to declare.

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