Dear Geoscientific Model Development Editorial Board, Dear reviewers,

Let me start by thanking both reviewers for their critical and constructive feedback on my manuscript. Both reviewers are quite critical on the ShellChron approach and raise valid concerns about its performance. Below, I will first attempt to summarize the main concerns raised by the reviewers and reply in general. Later, I will provide a point-by-point reply to the comments posed by the reviewers.

Firstly, I do not agree with Reviewer #2 that the model is oversophisticated and that it has no advantage over linear interpolation between seasonal extremes. As stated by Reviewer #1, there exist many seasonal archives with strong seasonal variability in extension rate (e.g. low-latitude bivalve shells). In most cases, approximating the seasonal curve through sinusoidal modelling, as is done by both ShellChron and the model by Judd et al. (2018), yields superior results over linear interpolation between seasonal extremes.

That said, the reviewers highlight several key characteristics in ShellChron's output which indicate either a lack of clarity in the explanation of the calculations or sub-optimal implementation of the model. The reviewers give helpful suggestions on how the explanation can be improved, for example by including a step-by-step guide through a simpler (lower resolution) example and clearer explanation of how the parameters of ShellChron (e.g. days per year and length of modelling windows) are defined. These issues can be solved through an update of the manuscript text.

Issues related to the implementation of the model include the underestimation of the seasonal temperature amplitude highlighted by both reviewers, the occurrence of "flat lines" in individual modelling windows and the occurrence of high-frequency variability in the modelled temperature and growth curve after weighing and combining results from multiple modelling windows. Issues pertaining to the shape and fit of individual modelling windows relate to the way the SCEUA algorithm is implemented, and how its starting parameters are set in ShellChron (see comment by Reviewer #1). The overall match of the model to the multi-year δ^{18} O curve depends on the combination of consecutive growth years and the recognition of year transitions in the model. Improving these aspects of ShellChron requires updates to the code, after which the examples in the manuscript have to be reproduced.

I will reply in detail to the comments raised by both reviewers below to highlight how I plan to respond to the review comments and improve the ShellChron code and the manuscript according to their suggestions.

Reviewer #1

In ShellChron 0.2.8: A new tool for constructing chronologies in accretionary carbonate archives from stable oxygen isotope profiles, de Winter presents a model for temporally aligning sclerochronologic data. The approach expands on the growth rate model of Judd et al. (2018), with three notable improvements: (1) a sliding window approach that allows for more continuous age transformation of multi-year records, (2) a modular code design that increases usability and flexibility of application (e.g., user-specified proxy-to-temperature transfer function), and (3) propagation of error and uncertainty.

In premise, the approach offers an innovative solution to a complex problem and promises to elegantly addresses the key limitations of previous growth models. However, after reading the manuscript several

times and going through the supplement, I am still left with several questions about the practical application of the approach, including but not limited to:

(1) Attenuated amplitude of the modelled isotope data: Why do the modelled curves seem to consistently underestimate the known isotopic range (e.g., Fig 3)? The manuscript explains that each window is designed to include at least one full year of growth (L238), meaning that at least one (if not both) seasonal extremes should be included in any given window. Additionally, the stated benefit of fitting a (linearized) sinusoid to the data in the window (in the depth domain) prior to iterating the temperature and growth rate functions is to set realistic starting parameters and bounds (L267-272). Given this, it seems the modelled isotope curve of each window should accurately capture the seasonal range of values. This point is illustrated in Fig. S1, which shows the known and weighted mean modelled isotope curves for the Texel high resolution scenario (Fig. S1A) and the residuals (Fig. S1B). Consistent with Fig. 3, the residuals are normally distributed and center at 0‰; however, they exhibit a non-random distribution, paralleling the seasonal signal – a direct result of systematically underestimating seasonal extremes. This is important as it not only detracts from the potential climatological and biological insights from the temperature and growth rate functions, it also leads to spurious intra-annual temporal alignment of the data.

This is a valid point. Indeed, ShellChron systematically underestimates the total seasonal amplitude in the data. The reason for this lies in the (weighed) averaging of overlapping model windows. As illustrated in **Fig. 3**, individual model windows are not very sensitive to single datapoints, causing a slight smoothing of the seasonal δ^{18} O curve. This effect is exacerbated by the weighing of the δ^{18} O data within model windows, which causes datapoints on the edge of the model window to have lesser influence on the shape of the modelled curve. This weighing is implemented to prevent outliers in the data to influence the model outcome. The downside of this design choice is that individual datapoints in the extreme seasons (especially clear in the Texel case) fail to draw the simulation to the recorded maxima and minima in δ^{18} O.

Another factor that may contribute to the poor fit quality of some model windows might be the freedom given to the SCEUA algorithm. Currently, the algorithm is set to stop optimization when function values (δ^{18} O) and model parameters do not change by more than 0.01% between consecutive model runs ("pcento" and "peps" parameters in the "run_model.r" function), and the model is limited to 10000 function evaluations ("maxn" in "run_model.r") to limit processing time. Since large δ^{18} O datasets and overlapping modelling windows cause full ShellChron runs to already take over one hour on a modern personal computer in the current setup (as noted by Reviewer #2), limiting processing time is valuable. The sinusoidal fit was implemented to help the algorithm to find better starting values and cause the SCEUA optimization to converge within the set parameters. However, I concur that the advantage of this sinusoidal fit may have been overestimated. I will implement an option in ShellChron for the user to set the constraints on the optimization algorithm manually and to switch the sinusoidal fit off. To evaluate if the limitations placed on the SCEUA algorithm and/or the use of sinusoidal fitting cause underestimation of the seasonal δ^{18} O amplitude, I will test a range of SCEUA settings with and without sinusoidal fit on a small test dataset and describe the results of these tests in the manuscript.

While the underestimation of the seasonal amplitude in δ^{18} O data does indeed dampen the seasonal cycle of the modelled temperature curve, it should not negatively affect the modelled age-depth relationship (as was recognized by Reviewer #2, see below). To test this, I propose to include details on the residuals of the age-depth model for the test cases (Case 1 and Texel, see **Fig. 3**) into the manuscript and discuss any systematic (seasonal) offsets in the age alignment of the δ^{18} O data that may result from underestimation of the seasonal δ^{18} O amplitude.

(2) **Number of growing days**: In looking through the supplement for the Texel high resolution scenario, more than 35% of the windows predict that the duration of growth captured by the isotope data in each window is less than 7 days (as per '*Day_of_year_raw.csv*'). Again, if each window spans at least one year and realistic bounds have been set for the temperature and growth rate functions, then why is growth condensed into such a short duration?

The reviewer refers to the "flat lines" in some individual modelling windows, where ShellChron fails to properly approximate the seasonal δ^{18} O curve (see following comment). This issue is related to the previous point raised by the reviewer, and likely results from either a poor choice of initial modelling conditions through the sinusoidal fit, or from overly restrictive parameters of the SCEUA algorithm. If not properly recognized and removed, these flat model results may be partially responsible for dampening of the seasonal δ^{18} O curve by the model, because they are included in the average of the modelled δ^{18} O curve. As stated above, I intend to test the effect of the sinusoidal fit and limits on the SCEUA algorithm to assess whether these parameters compromise the model fit. In addition, I will reevaluate the code to make sure that any remaining "flat" parts of individual modelling windows do not contribute to the average.

(3) **Shape of the modelled isotope curves in the depth and time domains**: Why do some modelled isotope curves exhibit high frequency variability (e.g., Window 3 of the Texel high resolution scenario; **Fig. S2**)? My understanding is that the modelled curves derive from the sinusoidal temperature function and the skewed sinusoidal growth rate function, both of which exhibit monotonic increases or decreases between their peaks and troughs. Are these wiggles a function of the weighting? If so, why is it not consistent across all windows? Also, as alluded to above, many of the windowed curves exhibit long flat lines at their start and/or end, indicating that the temperature and growth rate function bounds might be impeding a better fit. I suspect there might be an error in the Case 1 and Texel examples, as some of the concerns addressed above don't appear in the Coral, Oyster, and/or Speleothem examples. (Could the upper amplitude bound accidentally been set at Tamp/2 in these examples?) However, it is difficult to (a) ensure that I fully understand the methodology and (b) evaluate the fidelity and applicability of the approach while these questions linger.

Individual model simulation ("windows") are constrained by the two sinusoids and will therefore not exhibit high-frequency variability. On checking the supplementary file **SI7** from which the data in the reviewer's **Fig. S2** is obtained I discovered that the high-frequency variability only occurs in modelled δ^{18} O data from Window 3, and only in the high-resolution Texel dataset. None of the modelling window results from any of the tested datasets (see **SI7** and **SI8**) exhibit this variability, and I am afraid the incompatible data in Window 3 of the high-resolution test on the Texel data results from a copying error. My apologies for the inconvenience. I invite the reviewers to verify that no high-resolution variability occurs in the other window simulations, as indeed such variability cannot result from the combination of two sinusoids. I will provide a clean export of the raw results of the model on the highresolution Texel dataset after addressing the issues raised above.

Other general comments

• The manuscript would benefit from a detailed guided example. It is difficult to clearly and concisely convey complex mathematical model. Rather than presenting the Case 1 and Texel examples (which ultimately don't add much insight that can't be gleaned from the real-world examples), I would suggest

creating a shorter (<5 yearlong) virtual dataset and stepping the reader through 2 or 3 window examples, showing the temperature and growth rate functions for each window and comparing those to the known values.

This is a great suggestion, and I am happy to implement it in a revised version of the manuscript. From the review comments it is clear that the manuscript as well as the ShellChron package would benefit from a step-by-step guided example through the model using a realistic δ^{18} O record.

• It would be useful to address how the moving window approach is impacted by changes to the number of samples per year change and/or interannual extension rate. In practice, it can sometimes be difficult to sample at a constant rate and/or samples are sometimes lost or too small to run. How would the moving window approach adapt to an example where the first year had 15 samples and the second had only 8? Similarly, how are the results impacted if there is a large change to the interannual extension rate (as is observed in some low latitude bivalves)?

A good suggestion, and I would happily implement it by testing ShellChron on a more realistic (lower sampling resolution) virtual dataset with varying extension rate. Note that the Texel dataset currently implemented already features a decreasing extension rate, but I concur that it may be more interesting to test a more realistic δ^{18} O record with lower sampling resolution in which this decrease occurs.

• Can you please clarify whether the period of the window (in the time domain) is defined during the linearized sinusoidal fit or if it is fixed at 365 days?

The period of one year, as defined by the model outcome, is set at 365 days (although it is possible for the user to override this default through the "T_per" parameter). Window length is defined based on linear interpolation between the user provided YEARMARKERS such that each window contains at least one growth year. The length of a full window can therefore be longer than 365 days, as the length of one year in sampling direction is determined by the model outcome based on the δ^{18} O data. An initial value for the period in sampling direction is found through the sinusoidal fit before the SCEUA algorithm optimizes the growth rate and temperature sinusoids. These points will be clarified in the revised manuscript.

Line-by-line comments

L22: This notation is not defined until L70; I'd suggest rephrasing to 'oxygen isotope records'

I will rephrase this accordingly in the Abstract.

L39: Change 'time' to 'temporal'

I will rephase to "temporal"

L54: Delete 'of'

"of" will be deleted

L54: Change 'greenhouse warming' to 'anthropogenic warming' or something of the like – we're still a far way off from a true ice-free greenhouse climate

Agreed, I did not want to suggest that we are in a greenhouse state, rather refer to "warming by greenhouse gases". I agree that "anthropogenic (global) warming" is better and will rephrase accordingly.

L58: Change 'by' to 'at'

"by" will be rephrased to "at"

L71: Change 'by' to 'at'

"by" will be rephrased to "at"

L73: 'one being dominant over the other' – I'm not sure I completely agree; it can be quite difficult to disentangle these signals with, for example, low latitude, shallow bivalves and corals that are subject to seasonal precipitation; perhaps revise to 'with one generally being dominant over the other'

Agreed, I will rephrase to "with one generally being dominant over the other".

L91: Change 'causes them to rely on' to 'require'

I will rephrase to "requires"

L109: Define SCE-UA (Shuffled Complex Evolution model developed at the University of Arizona)

The abbreviation will be defined here.

L112: Sample trajectories are referred to as "depths" in the text of the manuscript but "lengths" in the figures (I'd suggest opting for "sample distance", as that term is more widely applicable ("depth" is an odd term in reference to bivalves)

This is a good point, and I will refer to "sample distance" or "distance in sampling direction" throughout the manuscript.

L138: Rephrase 'the question which'

I will rephrase to "Which carbonates are..."

L138 – 154: The original foraminifera references should be Spero et al. (1997) and Zeebe (1999). However, I'd contend that these studies do not suggest that foraminifera are precipitated out of equilibrium with their environment, but rather that additional environmental variables pertaining to the carbonate system (e.g., pH) contribute to oxygen isotope value of carbonate. This discussion is important (!) but highly nuanced, and I'm not sure this is the appropriate platform to address it. I'd suggest removing this section or moving it to the supplement; the important part of this paragraph as it pertains to the work presented in the paper is that ShellChron permits the user to define their desired transfer function.

I agree that this is not the place to discuss the equilibrium fractionation of foraminifera or the effects of environmental parameters on their δ^{18} O value. Therefore, this paragraph will be shortened, focusing on the importance of ShellChron's flexibility in choosing different transfer functions for the δ^{18} O-temperature relationship.

L162-163: Rephrase 'temperature evolution'

This will be rephrased to "the evolution of the calcification temperature"

L168: Change 'priory' to 'priori'

This will be rephrased accordingly.

L206 (and all other instances): I don't know that 'depth' is the correct word choice; bivalves aren't generally discussed in terms of a depth domain, but instead a sampling 'distance' along a growth axis See above, I agree and will refer to "distance (in sampling direction)" throughout the manuscript. L211,212: Change both instances of 'were' to 'are' for consistency of tense throughout the paragraph This will be rephrased for consistency.

L316: delete 'in the'

This will be rephrased to "Wadden Sea (North Netherlands; Texel; see details in...

Reviewer #2

The paper presents the details of ShellChron, an R package that calculates the inner chronology of seasonally resolved oxygen isotopic records such as those obtained from corals, mollusks or some speleothems. ShellChron does so by calculating a d18O curve combining an assumed sinusoidal temperature curve, a quasi-sinusoidal growth curve, and a paleo-temperature equation, fit onto the d18O record in moving windows. The performance of the model is evaluated using synthetic and real records.

While I acknowledge the importance of the inner chronology issue in the study of seasonal scale processes from paleoclimate records, ShellChron seems like a heavy oversophisticated solution (several hours of calculations per depth-age model) with no clear advantage compared to simple techniques like matching the d18O record with local temperature curve or a simple linear interpolation between seasonal isotopic extrema used as anchor points.

I agree that, in modern cases where local temperature and salinity curves are available, a modelling approach like ShellChron or the model in Judd et al. (2018) is not necessary, because the δ^{18} O data can be aligned to those known temperature and salinity curves. However, in cases where "true" environmental data are not available, modelling the seasonality curve has clear advantages over simple linear interpolation between seasonal extremes. As discussed in lines 82-97, in most shallow marine carbonate archives both temperature and growth rate describe quasi-sinusoidal patterns. Linear interpolation between maxima and minima (assuming constant growth rates in between) cannot approximate the growth rate in these records as well as a sinusoidal curve (see discussion in Judd et al. 2018). Therefore, in absence of "true" temperature and salinity records (i.e. in fossil archives), the sinusoidal modelling approach is a much better assumption for age-modelling than linear interpolation.

The author interprets too positively the test results. In my view, the tests indicate low performance in terms of dating precision despite the high quality of the records (synthetic or real), which questions the usefulness of the whole package.

In my discussion in relation to Figures 3-5, I honestly discuss the uncertainties of ShellChron in terms of reproducibility of the model result (precision) as well as agreement with the "true" age-distance relationship of the archive (accuracy). It is true that the ages found by ShellChron tend to have uncertainties of \pm 30 days or higher (see e.g. lines 345-361), but the advantage of ShellChron is that this uncertainty is known and quantifiable. In previous models, and especially when assuming constant growth between seasonal extremes (see above), this uncertainty is unknown. Furthermore, uncertainties calculated by ShellChron uniquely consider uncertainties in both the δ^{18} O measurement

and the sample position, making these uncertainties seem higher than those in other models. If the reviewer believes the discussion of ShellChron's uncertainty is insufficient, I invite any comments indicating where the results of ShellChron are interpreted too positively and how these improvements could be made.

- It is said in the text that a seasonally varying water d18O curve can be included but it is not clear how to do so in practice.

This is a valid point. In fact, the δ^{18} O cure can be provided as a vector object named "d18Ow" in the ShellChron functions within the R environment. I will make sure to mention this specifically on revision.

- A sinusoidal temperature curve is not a valid assumption in many tropical sites where the temperature annual cycle is bimodal. The growth curve is also a strong a priori assumption that cannot be tested. Growth parameters often evolves through ontogeny. Uncertainties estimated by the model do not include the uncertainty related to these assumptions.

These are all fair comments. I fully acknowledge that the sinusoidal temperature curve and skewedsinusoidal growth rate curves are approximations of reality. These approximations are discussed in detail in Judd et al. (2018), where they are first defended. In fact, the growth and temperature sinusoids are very flexible and can be modelled to a wide array of data shapes. Their use as target curves is therefore not a very restricting assumption. The fact that growth parameters evolve through ontogeny does not influence the accuracy of ShellChron, because each modelled window is independent. Growth parameters can (and will) change throughout the δ^{18} O record, and this change can be modelled by ShellChron. Indeed, there are situations in which the combination of sinusoids is not valid, and the tropical bimodal temperature seasonality is a good example. The reviewer therefore correctly highlights that ShellChron can only be used is archives where the sinusoidal δ^{18} O variability can be assumed to be annual. In reply to this comment, I will more clearly highlight this caveat of ShellChron in the revised manuscript.

- It is finally unclear whether ShellChron requires annual marker to be defined or not. While the text says it is not required (can be used with archives without annual markers), Figure 2 suggests otherwise, and it is not clear how the moving window size is determined if annual markers are not provided. If annual markers are provided, how is the uncertainty of this date dealt with?

This is a valid point, and I realize that this is not sufficiently clear from the text (see lines 233-241). In short, I tried to make ShellChron as independent from user-provided yearmarkers as possible. The yearmarkers in the input data are only used to constrain the minimum lengths the modelling windows require to contain a full year of growth. The sizes of the moving windows are determined at the beginning of the model routine (in the "data import" function) by linearly interpolating the distance between user-provided yearmarkers. After this step, the yearmarkers are not further used in ShellChron. This allows the model to freely assign the annual growth per window. This is one of the characteristics that distinguishes ShellChron from the Judd et al. (2018) model, which does use the yearmarkers to divide the δ^{18} O curve into annual chunks before running the model. In the revised version, I will make sure that the use of the yearmarkers is clearly explained.

- Figure 1 should be more explicit about input data and output data.

The figure already shows which data goes into the model and which comes out and illustrates the flow of pieces of data within and between functions in the model. To answer to the reviewer's comment, I will spell out the exported data types more specifically in the figure. I invite any suggestions on how to further specify details on input and output.

- Figure 2: "simulated parameters" should be defined more explicitely.

I will name the individual simulated parameters (e.g. " δ^{18} O", "temperature", "age", "SD on age", etc.) directly in the figure and caption.

- Tests are performed with very high resolution records (>23 datapoints per year), while the resolution in seasonally resolved records is generally limited to 10-12 datapoints per year for cost optimization reasons. The model should be tested with lower resolution records, in accord with real paleoclimate practice.

This is an excellent suggestion, and I will include an example of a lower resolution dataset to provide a more realistic benchmark for testing ShellChron. Note that real examples were already included in the study (see **Fig. 4**), but I concur that the sampling resolution in these cases is probably higher than average.

- Case 1 is almost an ideal case. Surprisingly, the standard deviation of the chronology is more than a month. It seems that a simple linear interpolation would yield a better precision.

Case one represents an ideal case in which growth rate does not vary seasonally or change along the record. In this special case, linear interpolation indeed outperforms the sinusoidal model, because the growth rate is constant. Unfortunately, such cases are rare (if they exist at all) in nature, so the fact that the linear interpolation outperforms the results of ShellChron does not disprove that sinusoidal modelling of δ^{18} O is superior to linear interpolation in natural cases. Note that the standard deviation on the chronology in ShellChron includes uncertainty on the optimization routine as well as on the measurements of δ^{18} O and the position of the sample (in sampling domain). In light of these uncertainties, it seems that an uncertainty of more than a month is realistic.

- Testing with case 1 and Texel presented in Figure 3 shows that the model produced by ShellChron systematically underestimates the annual cycle amplitude (in contradiction with the text which says that there is no systematic seasonal bias). This is not necessarily a problem for the depth-age model, but this is not supposed to happen based on the calculation description and points to a potential issue in the code.

I fully agree with this comment, and Reviewer #1 highlighted a few issues with the model that may cause this underestimation (see reply to their comments above). In short, I will experiment with the parameters restricting the SCEUA optimization, the use of the sinusoidal regression and the implementation of weights in averaging the overlapping model solutions to test whether the choice of parameters in ShellChron introduces artifacts on individual model simulations (e.g. flat lines on modelled δ^{18} O and dampened seasonal amplitude) which propagate into the model result. The results of these tests will be added to the revised manuscript. In addition, I will add a step-by-step guide through the model functions using a more common, low resolution δ^{18} O dataset to illustrate the effect of the

various modelling steps. Finally, I will discuss the effect of changing or introducing model parameters on the age-depth result and check model residuals for systematic offsets in ShellChron's age results.

- The model is doing poorly with the Texel case. The author acknowledges that errors occur because of monthly scale variability, which is actually what happens in the real world. The chronology of the Texel case would be accurately obtained with seasonal anchor points and linear interpolation. I have not entered into the code but it seems that it needs to be improved.

ShellChron indeed simulated a jump in the age-depth relationship for the Texel sample. Under normal circumstances, such a jump of one full year in the model could be easily detected and removed from the data (as discussed in lines 355-361) or amended by re-running the model. However, I decided to use this result to illustrate the types of issues the user could run into while implementing a model like ShellChron without proper supervision of the result.

In all cases in this manuscript, it is assumed that no environmental data is available. In analyzing the Texel dataset without *a priori* knowledge about the environmental temperature and salinity changes, linear interpolation between the only known anchor points (the seasonal δ^{18} O extremes) would yield less accurate results than ShellChron. Not only is the Texel case marked by seasonal changes in both temperature and salinity (and therefore δ^{18} O_w), but its growth rate also varies seasonally and decreases along the record. These nuances cannot be captured by linear interpolation between seasonal extremes, making sinusoidal models like ShellChron or the model in Judd et al. (2018) the better option.

- The author says in the text that the model can be used with speleothems, in contradiction with the testing which concludes that the performance is too low with the speleothem case.

The speleothem case is included as a worst-case example, and ShellChron's performance in this case is indeed low. However, in the discussion I highlight that age modelling in speleothems is possible in principle if the δ^{18} O record is good enough (see lines 181-184). I concur that these statements may come across as contradictory. Therefore, I will nuance my discussion of the application of ShellChron on speleothem records by more clearly stating the conditions these records should meet before results from ShellChron (or other sinusoidal δ^{18} O modelling) can be relied upon.

- In the test with real-world records, the performance of the model is evaluated using chronologies reconstructed using simple fit and interpolation method, which seems like an implicit acknowledgement that these simple techniques are superior.

Linear interpolation is only used to compare to the ShellChron results for the speleothem record (see **Fig. 4C**). The reason for this is that no sub-annual age model is available for this speleothem. By no means do I mean to suggest that speleothems grow through constant, year-round linear extension. In fact, drip water supply to (and therefore growth in) most speleothems varies seasonally (see Baldini et al., 2008; Van Rampelbergh et al., 2014; Vansteenberge et al., 2019; see lines 181-184 and lines 488-500). Therefore, sinusoidal models like ShellChron likely result in more realistic sub-annual growth rate reconstuctions than linear interpolation. I therefore think that the statement by the reviewer is not correct.