

NSF GEO Directorate

**Collaborative Research:  
GeoChronR – open-source tools for the analysis, visualization  
and integration of time-uncertain geoscientific data**

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**PROJECT SUMMARY**  
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**Overview**

Paleogeoscientists use natural archives to understand how climate, ecosystems, and environments varied prior to human monitoring. Accurately determining the age of samples is critical to this work, allowing scientists to pinpoint phase relationships between Earth systems and their forcings. Unfortunately, the lack of an accepted framework to represent and treat age uncertainties limits the broader applicability of such records. Over the past twenty years, the community’s approach to modeling ages in a depth sequence has become increasingly sophisticated, most recently resulting in Bayesian- and Monte Carlo-based approaches that more realistically characterize the full range of uncertainty and provide more robust estimates of age through a sequence. Because they are ensemble-based, these techniques allow for a quantitative evaluation of how age uncertainties affect quantities derived from such records. However, most domain scientists only use these tools to develop single, best estimates of age, and only qualitatively assess the influence of time uncertainties on their paleoenvironmental records. The proposed work will develop an integrated framework that allows scientists to generate state-of-the-art age models for their records, create time-uncertain ensembles of their data, analyze those ensembles with a number of commonly-used techniques, and visualize their results in an intuitive way. The code will be developed as a package in the open-source and community-supported R platform, facilitating broad dissemination.

Geochronologic data are rarely archived, and these software advances require a standard way of archiving time-uncertain data. We will use a universal, preliminary structured format that achieves this goal. As a proof of concept, the format will be applied to a data rescue effort with the World Data Center for Paleoclimatology, in a focused effort to recover primary geochronologic information for marine and terrestrial records of the Holocene, synthesizing and improving the archive resulting from the NSF Earth System History (ESH) Holocene initiative. These unified software and data standards will enable improved uncertainty quantification on the analysis of single records (the bread and butter of paleogeoscientists), multiproxy syntheses, and the integration of paleo data with dynamical models.

**Intellectual Merit**

Treating age models as an ensemble of many, equally likely, age-depth relationships, will enable paleogeoscientists to easily quantify uncertainties in their records of past climate, ecosystems or landscapes, and in quantities derived from them – without requiring special knowledge in data science. This will allow for:

1. More robust integration of time-uncertain records with precisely-dated layer-counted records (especially tree-ring chronologies) that are widely used to inform our understanding of the climate of the past 2,000 years (the Common Era);
2. Better understanding of abrupt climate changes (duration, spatial expression, synchronicity);
3. Improved integration of Earth system models with time-uncertain observations, allowing for a more rigorous tests of scientific hypotheses pertaining to model simulations of Earth’s past.

**Broader Impacts**

This project will create a powerful and ergonomic framework that will allow all paleogeoscientists to take full advantage of recent improvements in age-uncertainty quantification, and we will distribute these algorithms on the open-source and community-supported R platform. At present, no such tool exists, so the vast majority of paleogeoscientists leave this potential for insight untouched. Two workshops will ensure broad community feedback and the training of early career scientists in these new tools. This grant will also support two early-career scientists, a graduate student and up to four student interns.

# PROJECT DESCRIPTION

## 1 Objectives and Community Need

Quantifying chronological uncertainties is fundamental to the paleogeosciences. Without robust error determination, one cannot properly assess the extent to which past changes occurred simultaneously across regions or the duration of abrupt events, both of which limit our capacity to apply paleoscientific understanding to modern and future processes. The paleogeosciences community recognizes the need for a better infrastructure to both characterize uncertainty and to explicitly evaluate how age uncertainty impacts the interpretation of records of past climate, ecology or landscapes [Noren *et al.*, 2013]. In response to this need, the paleogeoscience community is making rapid advances toward improving geochronological accuracy by:

1. Improving analytical techniques that enable more precise age determination on smaller and context-specific samples [e.g., Brown *et al.*, 1989; Eglinton *et al.*, 1996; Eggins *et al.*, 2005; Santos *et al.*, 2010];
2. Refining our understanding of how past changes in the Earth system impact the age accuracy, for example: improvements to the radiocarbon calibration curve [Stuiver *et al.*, 1991, 1998] and advances in our understanding of spatial variability in cosmogenic production rates used in exposure dating [Balco *et al.*, 2009; Masarik and Beer, 2009];
3. Dramatic improvement in the level of sophistication and realism in age-depth models used to estimate the ages of sequences between dated samples [e.g., Heegaard *et al.*, 2005; Ramsey, 2009; Blaauw, 2010; Blaauw and Christen, 2011].

These advances allow for increasingly accurate ages and a more robust understanding of their uncertainties. Indeed, efforts in improving the accuracy and precision of geochronologic techniques are critical, and an area of community focus, as demonstrated by the NSF-funded EARTHTIME initiative<sup>1</sup>. However, the dynamic nature of geochronology makes intercomparison of recent work with prior studies that utilized now-obsolete standards very difficult. This problem is exacerbated by the fact that the vast majority (>90%) of archived records do not include the original geochronological information needed to update the age models and allow apples-to-apples comparison [cf., Renne *et al.*, 2009]. Recently, the lack of a mechanism for tracking changes in chronologies, and the lack of data standards in chronological data were recognized as "challenges to high-impact, interdisciplinary science" [Noren *et al.*, 2013].

### 1.1 The need for geochronology informatics

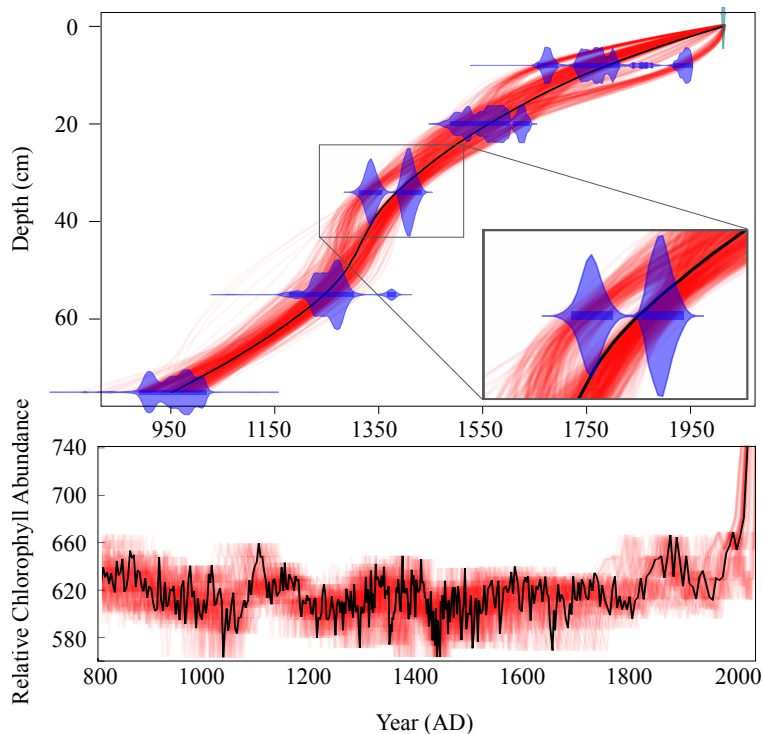
This problem is well-suited for an informatics solution. Age estimates for natural archives are dynamic, and would benefit from automation. Imagine a new study that updates our understanding of the age and geochemistry of a widespread ash layer. These changes would influence the geochronologies of other records. For some, the age of the tephra shifts slightly. For others, tephtras whose geochemistry did not match any potential records, now do. The updates to these chronologies may change what had previously appeared to be an asynchronous transition in a region, to a synchronous one. These changes would propagate to different records dependent on this chronological marker, perhaps fundamentally altering previous scientific conclusions. Such work would take many years with the current cyberinfrastructure, but would be feasible once integrated data structures and adapted software are developed.

Such a framework is beyond the scope of this proposal; although it's in line with many of the goals of the EarthCube initiative<sup>2</sup>. This proposal will leverage EarthCube activities, building upon advances in data standards and infrastructure intended to make geoscientific data more broadly useful for 21<sup>st</sup> century applications. Here we propose to develop and distribute GeoChronR, a one-stop shop to create, analyze,

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<sup>1</sup><http://www.earth-time.org/about.html>

<sup>2</sup><http://www.nsf.gov/geo/earthcube/>



**Figure 1:** Example of an age-depth model that corresponds to use case 1 (upper panel). The blue shapes illustrate the unique, often multi-modal, probability distributions of each of the calibrated  $^{14}\text{C}$  ages in the upper-most part of the core. Modern age-modelling algorithms typically account for this by deriving an ensemble of equally-plausible age models where each ensemble member fits a model through ages sampled from each date's probability distribution (red curves) [Blaauw, 2010]. These curves realistically diverge when passing through multi-modal ages; however these individual curves are rarely analyzed, rather the median of the ensembles (black line), which bisects bimodal distributions (inset) is used for all analyses. This impacts the interpretation of the record from the site (lower panel), where the impact of the trimodal peak, near 1900 AD, and the bimodal peak (near 1400 AD), are easily seen in the red ensemble curves, but not on the median age model.

visualize and integrate time-uncertain records. GeoChronR is well-aligned with the EarthCube vision; and the community-supported package may serve as a blueprint for grassroots development of analytical tools. Here, we propose two complementary efforts: one aims to make critical geochronologic data more accessible; the other will provide the tools to allow scientists to take full advantage of geochronologic information to better quantify past changes in the Earth system.

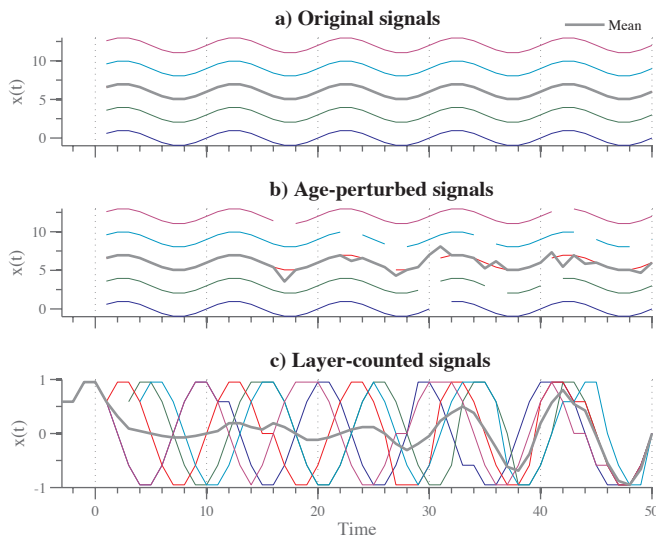
## 1.2 Three use cases for geochronology informatics

The proposed tools have a variety of target users across the paleogeosciences, ranging from scientists developing new records of past ecological change, to climate scientists trying to evaluate how well a climate model simulates a period of Earth's past. Here we provide three example use cases, demonstrating the breadth of the tools we will provide. Because of our background and research interests, the examples here, and throughout the proposal, are primarily focused on paleoclimatology. Nevertheless, many of these concepts and tools are directly applicable or easily extendable to other disciplines in the paleogeosciences.

### 1.2.1 Use case #1: Climate-proxy calibration with time-uncertain records

A paleolimnologist returns from the field. After measuring reflectance spectroscopy on the sediment cores to estimate down-core changes in chlorophyll content (an indicator of primary productivity in many lakes), and developing age control for the core with 17  $^{14}\text{C}$  dates, two tephra layers, and a  $^{210}\text{Pb}$  sequence near the surface, she would like to perform several tasks:

- create an age model to estimate ages and their uncertainties throughout the core (e.g., Fig. 1);
- visualize the reflectance data, along with a sense of how chronological uncertainties may affect individual wiggles;
- compare her series to that from a nearby lake. Her initial estimate of Pearson's correlation coefficient ( $\hat{\rho} = 0.43$ ) looks relatively high, but how much does this depend on chronological uncertainties in



**Figure 2:** Illustration of the distortion of coherent signals due to layer miscounting. (a) Five harmonic signals; (b) the same signals, sampled with a 5% chance of miscounting layers (missing years are shown in white); (c) the records assembled from (b) when assuming (erroneously) that 1 layer corresponds to 1 year. Note the loss of coherency between interannual signals from (a) to (c), and how strongly it affects the composite of those records (gray line). *GeoChronR* would enable to quantify the impact of such errors under plausible scenarios for the miscounting rate [from Comboul et al., in prep]

both records? She would like to quantify this uncertainty;

- calibrate her reflectance ratios to temperature from a nearby weather station via linear regression. The meteorological data are absolutely dated, her data are not. How much does this affect the range of regression parameters  $\alpha$  and  $\beta$ ?
- Perform spectral analysis and assess the significance of spectral peaks against an age-perturbed background. Although codes to perform optimal spectral analysis [Thomson, 1982] exist in R, Matlab and Python, no existing package allows to assess the effect of chronological uncertainties on such spectra.

An ensemble approach to age model development and record analysis, which is the core of *GeoChronR*, would enable her to simply perform all five tasks. It would also provide confidence intervals for  $\rho$ ,  $\alpha$  and  $\beta$  that quantify the effect of age model uncertainty.

### 1.2.2 Use case #2: Multiproxy reconstruction of tropical Pacific climate

In recent years, paleoclimatologists have shifted their emphasis from the analysis of single proxy records to large-scale syntheses involving many proxy types from all over the globe [e.g. Kaufman et al., 2009; Shakun et al., 2012; PAGES2K Consortium, 2013; Marcott et al., 2013; Tingley and Huybers, 2013]. To do so, one must grapple with chronological uncertainties that are highly heterogeneous in nature: some records are layer-counted, others dated via radiometric tie-points; all have disparate resolutions.

One important application is the reconstruction of past changes in tropical Pacific sea-surface temperature (SST). The equatorial Pacific, in particular, is home to the El Niño-Southern Oscillation (ENSO), orchestrating climate variability around the Pacific rim and throughout the global Tropics. Since there is evidence that the instrumental record is too short to adequately inform our knowledge of ENSO [Wittenberg, 2009], paleoclimatologists have sought to reconstruct its behavior from high-resolution proxy archives.

Recently, *Emile-Geay et al.* [2013a,b] used a network of 57 such proxies to reconstruct SST in the central equatorial Pacific (NINO3.4 region, [5°N–5°S; 170°W–120°W]) along with measures of uncertainty, exploring the results' dependence on the choice of proxy predictors, methodology, and instrumental target. Chronological errors are a key source of uncertainty that was not formally explored by *Emile-Geay et al.* [2013a,b]. How much would interannual oscillations (like ENSO) be affected by age offsets of just a few years between proxy predictors of very diverse types? How much would this propagate to estimates of low-frequency variability? Fig. 2 illustrates this concept. A proper framework to quantify the impact of such errors on ENSO reconstructions has heretofore been lacking, and would be enabled by *GeoChronR*.

### 1.2.3 Use case #3: Abrupt climate change and model-data intercomparison

The most recent preindustrial example of hemispheric-scale abrupt climate change occurred about 8,200 years ago [Alley *et al.*, 1997; Morrill *et al.*, 2013a]. Intervals of abrupt climate change are particularly relevant phenomena to investigate, both for advancing theoretical understanding of the Earth system’s capacity for extreme change, and for testing the climate models used for simulating future climate.

A paleoclimatologist has assembled a database of temperature and moisture records that span this interval, and is hoping to use these records to gain insight into the climate dynamics associated with the global-scale patterns in the database. The database includes a wide variety of archives with substantial differences in the types and quality of age-control; ranging from layer-counted ice cores with near-annual precision, to sediment sequences constrained by a few uncalibrated  $^{14}\text{C}$  ages. The predominance of evidence suggests that this abrupt event was associated with extreme freshwater forcing in the North Atlantic [Barber *et al.*, 1999; LeGrande *et al.*, 2006; Wiersma and Renssen, 2006; Carlson *et al.*, 2009; Hoffman *et al.*, 2012], however the underlying climate dynamics explaining the global-scale pattern of changes are not fully understood. The scientist would like to use these data to test between competing hypotheses: Were the climatic changes observed throughout the world primarily carried by atmospheric, or oceanic teleconnections, or some combination of the two? She’d like to test this by examining spatial patterns of the timing of onset and termination, as well as the duration of the event. Far distant sites, where abrupt changes start and end synchronously with records from the North Atlantic, were most likely forced by atmospheric teleconnections [Liu *et al.*, 2013; Morrill, 2013], whereas those whose response lags by several years or decades may be better explained by associated changes in ocean circulation [e.g., Cremer *et al.*, 2007; Ljung *et al.*, 2008]. The paleoclimatologist would like to:

- develop appropriate ensemble age-models for each record, using the most recent radiocarbon calibration curve and state-of-the-art age modelling techniques;
- rigorously and objectively identify the timing of onset, duration and termination of abrupt changes within range of the 8.2 ka event for each of 1000 equally-likely timeseries derived for each record;
- map the time-uncertain probability distribution for onset, duration and termination, for both temperature and precipitation;
- compare these results with climate model simulations to investigate the underlying dynamics.

We propose to make this effort possible by recovering and standardly formatting datasets relevant to this interval that will integrate easily with `GeoChronR`: a package of tools that allow robust age-model development, changepoint analysis of time-uncertain ensembles, and intuitive visualization routines.

## 2 Background

### 2.1 Age-Depth Modeling

The majority of archives used in the paleogeosciences are not annually-distinct. Consequently, to estimate the deposition (formation) time of different sections of a sequence, researchers directly estimate the ages of a small number of samples through the sequence (e.g., Fig. 1). These are often radiometric estimates, such as  $^{14}\text{C}$ , which is common for lake or marine sediment records, or U-series dating in speleothem or coral records. Often, chronostratigraphic markers, such as ash layers deposited after volcanic eruptions of known ages, or other distinct changes or events in a record which are tied to age in other records. These age estimates provide a general overview of how age changes as a function of depth or distance, but considerable uncertainty remains about how to estimate ages for samples between the directly estimated layers.

Generally speaking, the paleogeoscience community has gradually shifted from simpler to more complex approaches to this problem. Simple solutions, such as fitting a least-squares regression line through the ages, or linearly-interpolating from age-to-age have been long used [cf., Bennett, 1994], and remain

extremely common; a literature survey for 2008 showed the majority of studies used one of these two types of models [Blaauw, 2010]. Each of these approaches has its pros and cons. The linear regression approach treats errors very conservatively, but does not allow for changes in sedimentation or accumulation rate, and cannot take full advantage of well-dated layers. Piecewise linear interpolation may be the most conservative way to estimate ages between two control points, but implies abrupt changes in sedimentation rate at the age points, and it is difficult to estimate uncertainty in the model – doing so with ensemble methods suggests that the mid-points between ages have the least uncertainty, which is counterintuitive.

To address these issues, techniques that model slow changes in accumulation rate but that curve to fit through age control points are being adopted. In these models, polynomials or splines were fit to the age control points. These models have the opposite implications on the timing of sedimentation rate changes, spreading them over the gaps between points while minimizing changes at the control points. It remained unclear, however, how to estimate uncertainty for these models. To this end, algorithms were developed to estimate uncertainty for spline-based models. Heegaard *et al.* [2005] published a mixed-effect regression model that estimates uncertainty in the spline fit by combining the uncertainties originating from the analysis of each dated layer as well as the variability between dated layers. Thus, records with more variability in sedimentation rates resulted in broader error bars than did monotonic records. Blaauw [2010] took a different approach, calculating an ensemble of age model splines by iteratively sampling from the full error distribution of each age, then fitting a spline through each age. This allowed for realistic examination of how the irregular error structure of calibrated radiocarbon ages influenced age models (Fig. 1).

Most recently, Bayesian approaches have been employed to age-model development [Blaauw and Christen, 2005; Ramsey, 2009; Blaauw and Christen, 2011]. These algorithms are able to incorporate a more realistic understanding of how geologic sequences accumulate. To date, this has been done via statistical estimates of probability distribution and autocorrelation structure of accumulation rates [Ramsey, 2009; Blaauw and Christen, 2011; Ault, 2011; Comboul *et al.*, in prep]. Future work may improve on this approach by including biogeochemical models that simulate these processes.

## 2.2 Time-uncertain analysis

Despite the progress made in quantifying uncertainty in ages and in age models, few studies have formally evaluated how chronological uncertainty may have affected their results. For instance, whereas the algorithms presented by Heegaard *et al.* [2005] and Blaauw [2010] have been broadly used in the paleolimnology community, the overwhelming majority of these studies calculate the single best-estimate model (often a median or mean), use this model to put measured paleoclimatic or paleoenvironmental data on a timescale, and then proceed to analyze the record with little or no reference to the age modeling exercise [e.g. McKay *et al.*, 2008; McKay and Kaufman, 2009, and many others]. Typically, discussions of the impact of chronological uncertainties remain qualitative.

Thankfully, this paradigm is beginning to change. In recent years a handful of studies have taken advantage of approaches that generate ensembles of age models to evaluate how the results of their analyses and conclusions vary given differences between ensemble members [Haam and Huybers, 2010; Rhines and Huybers, 2011; Anchukaitis and Tierney, 2012; Shakun *et al.*, 2012; Marcott *et al.*, 2013; Tierney *et al.*, 2013]. By using each ensemble age model to create a time-uncertain ensemble records, and then carrying that ensemble through the analysis, the precise impact of age uncertainty can be formally evaluated. This approach, of course, does not address all aspects of uncertainty, but it does offer the broad potential to ascertain which results are robust to chronological uncertainty, and which are not.

Despite its potential to substantially improve uncertainty quantification for the paleogeosciences, this framework is not widely utilized. The majority of studies using this approach have been regional [Anchukaitis and Tierney, 2012; Tierney *et al.*, 2013] or global-scale [Shakun *et al.*, 2012; Marcott *et al.*, 2013] syntheses, or reanalyses of well-known datasets [Haam and Huybers, 2010; Rhines and Huybers, 2011]

rather than primary publications of new records. There are likely several reasons for the lack of adoption of these techniques:

- The necessary geochronological data are not publicly available for the vast majority of records. Even when they are available, the data are archived in diverse and unstructured data formats. Together, this makes what should be a simple process of aggregating and preparing data for analysis prohibitively time-consuming;
- Few tools for ensemble analysis are available, and those that are require a degree of comfort with coding languages and scientific programming that is rare among paleogeoscientists;
- There is a disconnect between age-model development and time-uncertain analysis. Published approaches have utilized either simplified age-modeling approaches [Haam and Huybers, 2010], or specialized approaches not used elsewhere in the community [Shakun *et al.*, 2012; Anchukaitis and Tierney, 2012; Marcott *et al.*, 2013; Tierney *et al.*, 2013]. Currently, extracting the relevant data from commonly-used age-modelling algorithms, creating time-uncertain ensembles, then reformatting those data for analysis in available tools is exceedingly technical;
- Finally, the proliferation of age-modelling approaches and analytical techniques has not been accompanied by a thorough intercomparison of the underlying theory, assumptions and biases associated with each approach. Consequently, it is difficult for most users to make informed decisions about how to model age and age-uncertainty for their records, and how their choices might influence their analytical results.

We will lower the barriers to broader adoption of these emerging methods by recovering, formatting and publicly archiving geochronological data, and by developing an easily-accessible, open-source software package of industry-standard and cutting-edge tools that provides users with a one-stop shop to create, analyze, and visualize time-uncertain data.

### 3 Recovering and formatting geochronological data for broad use

The primary focus of this proposal is to develop a set of software tools that will make emerging concepts in time-uncertain data analysis more broadly accessible. Nonetheless, software design is inevitably predicated on a consideration of data structures. The lack of a standard paleoclimate database archiving primary chronological information is therefore the first hurdle to overcome. To begin to address this issue, we will collaborate with the National Oceanic and Atmospheric Administration's World Data Center for Paleoclimatology<sup>3</sup> (WDC-Paleo, see letter of collaboration) to collect, aggregate and standardly format a broadly useful dataset. As of result of these efforts, we expect to have, for the first time, a Holocene terrestrial and marine dataset in a broadly useful format with fully-archived geochronologic data necessary for state-of-the-art analyses.

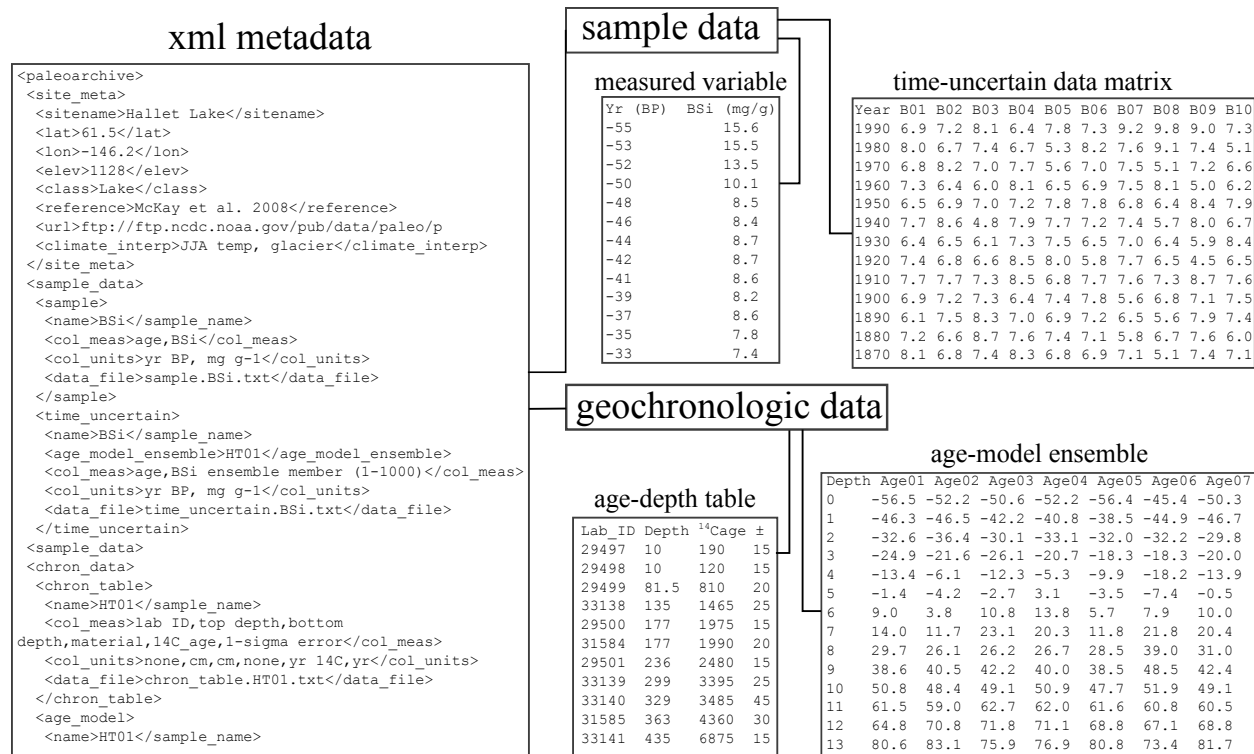
#### 3.1 Data format

At present there is no agreed-upon standard to publish, distribute and re-use paleogeoscientific data. This is partially due to the wide diversity of data types. To accomodate this diversity while maintaining a structured and searchable format, we will adopt the flexible approach proposed by *Emile-Geay and Eshleman* [2013]. Here, each record is described by a metadata file, written using the eXtensible Markup Language (XML), that describes all of the relevant metadata fields, and also points to text files which contain the tabular data associated with each record, indexed by depth (Fig. 3). There are two basic types of tabular data, sample data (e.g., physical, biological or chemical measurements used to infer past environmental variability)

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<sup>3</sup><http://www.ncdc.noaa.gov/paleo/paleo.html>





**Figure 3:** Schematic representation of the data structure to be used for GeoChronR.

and geochronological data. There are also two main types of chronological data: age-depth tables, describing best estimates of the age of dated layers, and the associated analytical data used to produce those estimates (e.g., fraction of modern carbon, for <sup>14</sup>C dates), and age-model data, which could either entail a best-estimate and error bounds derived from an age-modelling technique, or a large matrix with an ensemble of equally-plausible age-depth relationships, as in Fig. 3. These age-model ensembles will be used in GeoChronR to create time-uncertain variable matrices as input for time-uncertain analyses which require regularly-spaced data (see section 4.2 for details). Data recovered and formatted for this project will utilize this data structure. This is an important component of this research, and will make the geochronology data gathered for this proposal broadly useful for other applications as well. If and when the community agrees upon a standard format, conversion between our format and a new format will be straightforward, as any new standard must be self-describing and machine-readable.

### 3.2 A Holocene Climate Database

In collaboration with WDC-Paleo, we will update and combine existing compilations with well-formatted geochronological data, and recover missing geochronological data for other relevant records in the WDC-Paleo archive to create a well-structured database of Holocene climate data that will integrate smoothly GeoChronR. WDC-Paleo has extensive marine and terrestrial data contributed by investigators funded under the ESH Holocene initiative. Unfortunately measured age information is lacking, but will be recovered as part of this proposal. We chose the Holocene, the current period of warm climate following the end of the last Ice Age, about 11,500 years ago, as the target for this data recovery and formatting project for two reasons:

1. To move towards the long-term goal of expanding our understanding of Holocene and especially late Holocene climate reconstructions. Reconstructing spatial patterns in climate variability during the past several thousand years is an important component of improving our understanding of long-term

climate dynamics. This in turn informs estimates of how anthropogenic climate forcing may impact the climate system on these timescales. Our knowledge of the climate of the past two millennia is primarily derived from annually-banded paleoclimate archives; especially tree-ring records. Tree-ring records have several limitations however, primarily in that they rarely extend more than 1,000 years, and they typically can't capture the full range of low-frequency climate variability [Cook *et al.*, 1995]. Marine and lacustrine sediments, speleothems and ice cores are well-suited to both longer records, and for recording low-frequency variability, but are difficult to integrate with tree-ring and other annually-resolved records, largely due to the time-uncertainty associated with radiometrically-dated archives [cf., *Anchukaitis and Tierney*, 2012]. As detailed in use case #2, a readily usable database of Holocene paleoclimate records [Emile-Geay *et al.*, 2013a] will allow for a rigorous investigation of how time-uncertainty may impact a climate reconstruction of NINO3.4 SST for the past millennium.

2. To improve our knowledge of abrupt climate change. Use case #3 details how a well-structured database that includes all of the relevant geochronological data could be combined with `GeoChronR` to evaluate the spatial patterns of the timing of the 8.2 ka event in a probabilistic sense. Such an analysis would improve our theoretical understanding of how the Earth system can respond to abrupt climate change, and provide richer proxy benchmarks for data-model comparison [Morrill *et al.*, 2013b]

We will begin building this Holocene Climate Database by reformatting and, when necessary, recovering the geochronologic data from recent syntheses [Emile-Geay *et al.*, 2013a,b; Marcott *et al.*, 2013; Morrill *et al.*, 2013a]. These syntheses are excellent starting points for our data collection and formatting efforts since they are of broad interest, relevant to scientific questions described above, and in many cases, have already aggregated the original geochronological data. Subsequently, we will work with WDC-Paleo to expand the database, targeting Holocene records that are particularly relevant for integration with late Holocene climate reconstruction, and for better understanding the spatiotemporal pattern of abrupt change.

### 3.3 Distributing these data

By the initial release of `GeoChronR`, at a minimum, the uniformly formatted Holocene Climate Database will contain all the records from [Emile-Geay *et al.*, 2013a,b; Marcott *et al.*, 2013; Morrill *et al.*, 2013a], including all of the relevant geochronological data, and will be available as a standardized package at WDC-NOAA that will interact smoothly with `GeoChronR`. In addition, should our data aggregation and formatting efforts proceed as planned, dozens of additional records will also be included. The data contribution is critical, because the potential of examining these data with the time-uncertain analysis tools in `GeoChronR`, and for comparing new records with data in these archives will be the primary motivation for community adoption of `GeoChronR`. Ideally, these data will serve as a seed that motivates the formatting and inclusion of other records by users of `GeoChronR`, and spark community-wide discussion on data/metadata standards.

## 4 `GeoChronR` : an integrated, open-source and community-supported solution

We will develop a package in the R environment<sup>4</sup> that will link new and emerging age-modeling algorithms with analytical tools that allow users to analyze time-uncertain ensembles with several industry-standard and cutting-edge tools, and then effectively visualize those results.

A key aim of this effort is to increase community participation in a powerful new approach to understanding how geochronological uncertainty influences the associated records. Relatively few paleogeoscientists program in R, though it has been widely used for age-modeling algorithms [Heegaard *et al.*, 2005; Blaauw, 2010; Blaauw and Christen, 2011] and paleogeoscientists have proven themselves proficient at utilizing

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<sup>4</sup><http://www.r-project.org>

well-designed packages. Furthermore, R is open-source, freely-available, and is supported by an active community that contributes to packages. We will embrace this spirit and will encourage users comfortable in R to contribute new components to the package, especially community-specific analyses that can be simply expanded to analyze time-uncertain records. Indeed, many of the common analytical tools that we will develop for `GeoChronR` are modified versions of packages already contributed by the R community. We will also strive to accommodate users who prefer to work in other environments, working with the community to develop input and output routines that facilitate the interface between Excel<sup>TM</sup>, Matlab or Python.

## 4.1 Age Modeling tools

### 4.1.1 Tie-point age models

The CLassical Age Modeling (CLAM) algorithm [Blaauw, 2010], is designed to improve spline-based age modeling techniques by randomly sampling from the full age distribution of each age control point before fitting a spline through control points. Critically, CLAM calibrates each radiocarbon age and draws <sup>14</sup>C age estimates from each date's unique error distribution. CLAM can optionally exclude ensemble members with age reversals, enforcing the constraint of superposition, as well as handle downcore variability in <sup>14</sup>C reservoir corrections for marine records. CLAM is written in R, is ensemble-based, and is widely used, making it ideal for `GeoChronR`.

The Bayesian ACcumulation (BACON) algorithm [Blaauw and Christen, 2011] was designed as a Bayesian alternative to CLAM. Rather than utilizing purely statistical approaches to filling the gaps between ages, BACON is designed around the philosophy of taking advantage of prior knowledge about the distribution and autocorrelation structure of sedimentation rates in a sequence. The algorithm employs an adaptive Markov Chain Monte Carlo algorithm that allows for Bayesian learning to update the sedimentation rate distribution. BACON is written in C++ and R, with an R interface. A subset of ensemble members with high *a posteriori* probabilities can be extracted and used for ensemble analysis.

Ault [2011] developed an alternative method for utilizing prior knowledge about accumulation rate distribution to infer the ages of gaps between known ages. The age modeling component of Monte carlo Age model Families for Interpretation and Analysis (MAFIA) was designed to model ages for speleothem records, but is easily generalized to other archives. MAFIA simulates the intervals between dated layers as a random walk process whose steps are drawn from a gamma or Poisson distribution that is characteristic of the archive. Because age uncertainty is thought to be greatest at the mid-points between dated layers [Huybers and Wunsch, 2004], MAFIA simulates ages in both increasing and decreasing directions from each control point, stitching individual ensemble members together at the midpoints where uncertainty is greatest. MAFIA is coded in MATLAB, and will be adapted to R for this project.

### 4.1.2 Layer-counted age models

Another major dating technique exploits the presence of distinct bands or periodic features (e.g. cycles in geochemical measurements), whose count is equated with the number of years elapsed since the top sample was collected. This category covers tree-rings, varved sediments, ice cores and annually-banded corals. Dendrochronology is an extremely well-developed field, and cross-dating between many samples makes tree-ring chronologies extremely robust [e.g. Douglass, 1941; Stokes and Smiley, 1996]. Uncertainty quantification for the less time-certain archives (varved sediments, and annually-banded ice cores and corals), is much less developed. Rhines and Huybers [2011, Appendix A] proposed a simple model for long ice-core chronologies like that of GISP2 [Alley *et al.*, 1997]. Uncertainties are modeled as a discrete random walk, but in order to obtain relative uncertainties consistent with published estimates of 2%, they had to specify an unrealistically high probability for the miscounting of layers.

Recently, Comboul *et al.* [in prep] proposed BAM (Banded Age Model), a probabilistic model of age errors in layer-counted chronologies. The model allows a flexible parametric representation of such errors (either as Poisson or Bernoulli processes), and separately considers the possibility of double-counting or

missing a band. The model is parameterized in terms of the error rates associated with each event, which are more intuitive parameters to paleogeoscientists. Although such rates can be difficult to estimate from the data alone, field scientists typically have expert knowledge that can be tapped to refine these error estimates. Additionally, an optimization principle may be used to identify a more likely age model when a high-frequency common signal can be used as a clock. BAM is coded in MATLAB, and will be adapted to R for this project.

#### 4.1.3 Unifying the mathematical description of age errors

As is now becoming apparent, many approaches have been proposed to generate ensembles of chronologies based on tie-point or layer-counted age models. Some of these approaches make the underlying stochastic model explicit, others do not. Few have made their code publicly available. One task of this project will be to unify the mathematical description of age models, so that the merits of competing approaches can be more readily appraised. We will also perform comparisons on synthetic benchmarks, so that the advantages and disadvantages of each model and method can be made more transparent. The results of this work will be summarized in the tutorial for `GeoChronR` as well as in the interactive help, to help end-users decide which age modelling algorithms and methodological choices are most appropriate for their problem.

### 4.2 Ensemble Analysis and Visualization

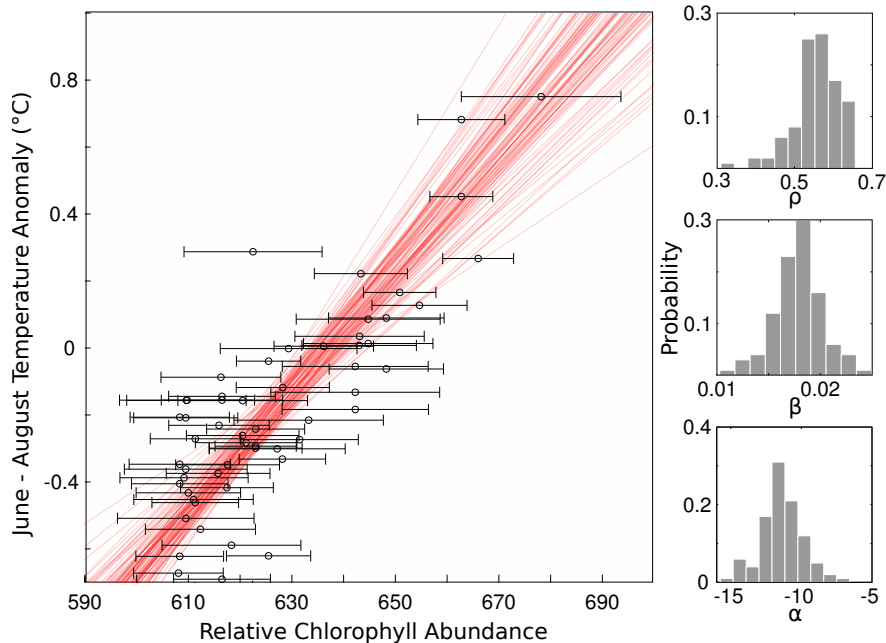
After the development of an ensemble of age models with one of the age modeling algorithms described above, the next step is to create a time-uncertain ensemble of a record of interest. This will be handled simply in `GeoChronR`, by using each age-model ensemble as a simple look-up table to convert depth to age using each ensemble model. This results in a matrix of ages (an “age-model ensemble”) that correspond to measured layers in the record. For some analyses, irregularly-spaced data may be analyzed. Many, however, require regularly-spaced data. For these, each age-value pair will be used to resample the data, by averaging the data over contiguous intervals, and where necessary, interpolating records to create a matrix with uniformly sampled age steps (the “time-uncertain data matrix”).

Visualization is an important component: the analysis of time-uncertain ensembles introduces an additional dimension to the results, meaning that traditional methods for visualizing many analyses will need to be enhanced to show the distribution of results across age-ensemble members. For each analysis included in the toolbox, we will develop one or more methods of visualizing the results and their uncertainty.

#### 4.2.1 Time-series analysis

Estimates of correlation and covariance are widely used in the paleogeosciences to evaluate the extent to which two time series are related, and to thus provide insight into the processes that may be driving covariability (or the lack thereof). Such analyses allow for an estimate of uncertainty, but the impact of chronological uncertainty cannot be easily assessed. [Haam and Huybers, 2010] developed a procedure to test the statistical likelihood that two timeseries are significantly covariable, given uncertainty in the chronologies. The authors show that evaluating the likelihood of significant covariance using a Monte Carlo based test is consistent with analytical results derived from the theory of order statistics. The authors use a sophisticated approach to evaluate the likelihood of the few ensemble members with the highest covariance, while using a simplified age-modeling scheme. We propose an alternative approach, where the ensembles are extracted from one of the approaches described above, but where the covariance of correlation statistics are calculated across the time-uncertain ensembles of two series (e.g., Fig. 4). The distribution of  $p$ -values, indicative of significance, are also calculated. This gives users an appropriate sense of the influence of chronological uncertainty on the statistical relationship between two records.

Increasingly, radiometrically-dated paleoclimate records are being calibrated against instrumental climate data to quantify past variability in temperature [e.g., McKay et al., 2008; Saunders et al., 2013], precipitation [e.g., Trachsel et al., 2010; Elbert et al., 2012; von Gunten et al., 2012] or discharge [e.g.,



**Figure 4:** Example of age-uncertain proxy calibration, following use case 1. Here, each age ensemble member is used individually to put the relative chlorophyll abundance data on a timescale. Next, each ensemble member is regressed against a nearby instrumental record to develop a calibration with summer temperature. The impact of age uncertainty on apparent chlorophyll abundance data is illustrated by the horizontal error bars on the left panel, and the regression lines resulting from each of 100 age-ensembles are shown in red. To the right, the probability distributions of  $\rho$ ,  $\beta$  and  $\alpha$  characterize the impact of age uncertainty on the calibration.

[Kaufman *et al.*, 2011] at a study location. Time-uncertainty in these records creates additional uncertainty in the calibration to climate that is typically ignored, but that could be simply evaluated by performing the calibration step (usually some form of regression), over an ensemble of time-uncertain predictors (Fig. 4). The calibration for each ensemble member will then be applied throughout the record to form a time-uncertain ensemble of the quantitatively reconstructed climate parameter that encompasses the influence of time uncertainty on the calibration procedure.

Traditionally, the influence of chronological uncertainty has been judged qualitatively, with the eye as a primary tool. This sort of judgment is much more difficult for analyses in the spectral domain, where the primary focus is to identify statistically-significant periodicities in a timeseries.

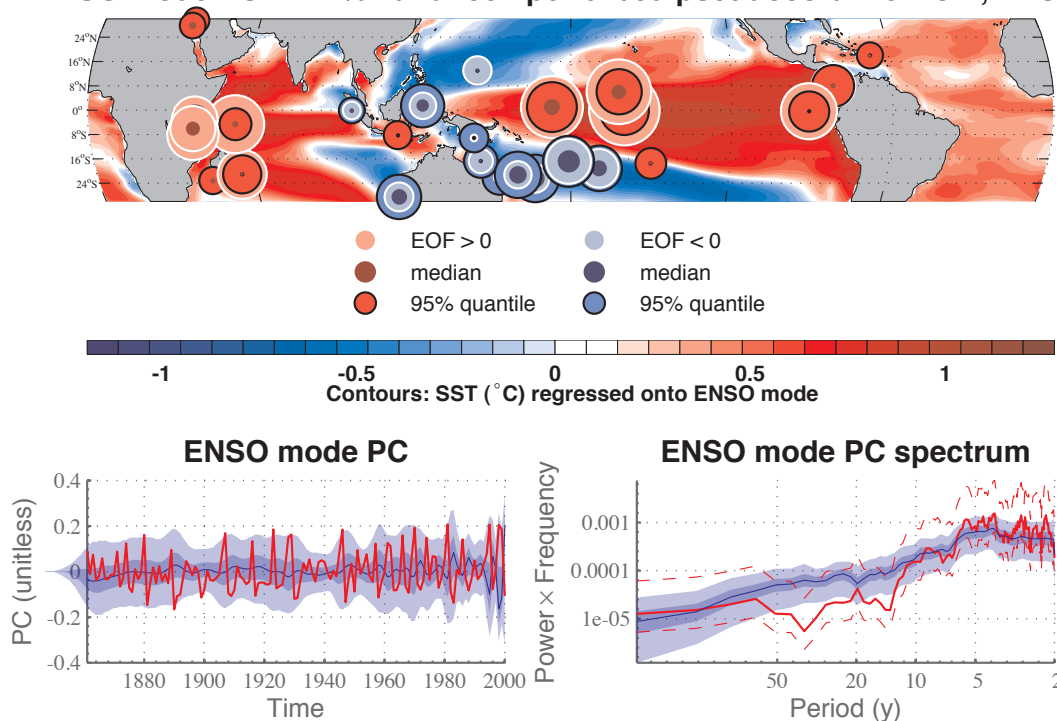
Thus, ensemble analysis in the frequency domain has the potential to be particularly enlightening. We will develop algorithms to calculate and visualize ensemble spectra and evolutive spectra for both regularly-spaced records using the multi-taper method [Thomson, 1982; Mann and Lees, 1996] as in [Comboul *et al.*, in prep] (e.g., the bottom right panel in Fig. 5), and for irregularly-spaced records using the Lomb-Scargle method [Schulz and Mudelsee, 2002; Mudelsee *et al.*, 2009]. We will also adapt R packages for wavelet and wavelet coherence analysis for ensemble analysis and visualization.

Many other types of time-series analysis methods can be adapted to apply to time-uncertain ensembles. For example, trend analysis [Santer *et al.*, 2000; PAGES2K Consortium, 2013], changepoint detection [Lund *et al.*, 2007; Reeves *et al.*, 2007; Ruggieri and Lawrence, 2012], and regime-shift tests [Rodionov, 2004; Morrill and Jacobsen, 2005] are widely used, and these will be developed for specific scientific questions as needed. We aim to create an environment that is so useful that technically-adept users interested in a specific analysis will contribute to a community-supported library of analysis functions.

#### 4.2.2 Spatiotemporal data analysis

Recently, Anchukaitis and Tierney [2012] presented a new approach to isolate, and evaluate the uncertainty of, shared regional patterns in time-uncertain data. Monte Carlo Empirical Orthogonal Function analysis (MCEOF) employs the same philosophy as GeoChronR; calculating ensemble age models and time-

### ENSO mode EOF - 27% variance - perturbed pseudocoral network, 27 sites



**Figure 5:** Spatiotemporal uncertainty quantification on a pseudocoral network. (top) EOF loadings (circles) corresponding to the ENSO mode of an ensemble of age-perturbed pseudocoral records with miscounting probability  $\theta = 0.05$ . EOF loadings for error-free data are shown in light colors circled in white, while the median and 95% quantile are shown by dark disks and black-circled disks, respectively. Contours depict the SST field associated with the mode's principal component PC (bottom left), whose power spectrum is shown on the bottom right. Results for the time-uncertain ensemble are shown in blue: median (solid line), the 95% confidence interval (light-filled area) and interquartile range [25%-75%] (dark-filled area). Results for the original (error-free) dataset are depicted by solid red lines. Dashed red lines denote  $\chi^2$  error estimates for the MTM spectrum. [from Comboul et al., in prep]

uncertain proxy records, then performing singular value decomposition on many equally-plausible matrices of multiple records for a region. The resulting empirical orthogonal functions, and their projections onto the time-uncertain records, yields maps of the EOF loadings, along with their uncertainties, and the corresponding principle component time-series which extract primary modes of variability that are robust to chronological uncertainty, with variable uncertainty in time. Comboul et al. [in prep] have implemented a similar analysis in MATLAB, with a visualization scheme inspired by that of Tierney et al. [2013, their Fig. 1c], presented in Fig. 5. Additionally, the lower-right panel illustrates one strategy for the spectral analysis of time-uncertain records. This technique will be applied in GeoChronR, leveraging other spatiotemporal analysis techniques like independent component analysis [Comon, 1994]<sup>5</sup> and multichannel SSA (M-SSA) [Vautard et al., 1992].

One unique outcome of GeoChronR, which will synthesize different age model representations under one unified informatic framework, is to enable the integration of time-uncertain records with a wide range of age precisions and chronological types. This is critical to the climate field reconstruction (CFR), which aims to reconstruct climate variability at high and low-frequencies from such heterogeneous datasets, and

<sup>5</sup><http://cran.r-project.org/web/packages/fastICA/index.html>

has yet to incorporate age uncertainties in its inference framework. The investigation of age uncertainties in CFR is beyond the scope of this proposal, but this work is a necessary step in this direction.

### 4.3 Data-model intercomparison

As evoked in use case #3, a key motivation for studying Earth’s past is the ability to test predictive Earth system models, by providing a completely independent set of observations that were not used for model development or tuning [Schmidt, 2010]. However, data-model comparisons are fraught with many difficulties. The first is that models and data do not speak the same language, so some form of translation must take place: either the proxy data are converted into a dynamically-relevant variable (e.g. temperature, precipitation) by means of an inverse technique, or model output is mapped into proxy space via proxy system models [Evans *et al.*, revised]. The second, of course, is that this comparison must be done in the presence of age errors.

There is no standard way to carry out such analyses; like all science problems, they must be tailored to test specific hypotheses. A good paradigm for paleoclimate data-model intercomparison is the PMIP3 initiative [Braconnot *et al.*, 2012], which provides a standard test of numerical experiments that can be confronted to paleoclimate benchmarks. For instance, the NINO3.4 reconstructions of *Emile-Geay et al.* [2013a,b] were used by *Ault et al.* [accepted] to constrain model behavior in the spectral domain. Much more can be done on this front [e.g. *Emile-Geay*, 2013], including explicitly recognizing time uncertainties in the proxy archives. Using our age modeling tools (4.1), we will develop R code to formally test the hypothesis that simulated behavior in perturbed experiments is compatible with time-uncertain proxy observations, and statistically distinct from that of control simulations. Two case studies will demonstrate use on 1) transient simulations of the last millennium (LM), as in *Ault et al.* [accepted], and 2) experiments targeting the 8.2 ka “event”<sup>6</sup>.

The first will explore the ability to distinguish spectral regimes in the presence of time uncertainties (a continuum approach); the second will quantify how much age uncertainties limit the resolution of abrupt climate changes, and hence how stringent a test they provide to climate models (an event-based approach).

### 4.4 Code development and publishing in R

GeoChronR will be developed as a package in R. The R programming ecosystem is a community-driven open source development framework derived from the statistical programming language S. R is freely available under the GNU general public license (GPL), and has an active base of developers contributing enhancements to R’s visualization, statistics, and machine learning capabilities. The capabilities of R are extended through user-created packages, which enable specialized statistical techniques, visualization methods, reporting tools, data ingestion mechanisms, and more. The Comprehensive R Archive Network (CRAN) is an open repository of these user-created packages, and presently contains 4638 contributions to the collection. Code is typically written in R, but may also be written in Java, C, Fortran, or others. Because of the open nature of R and CRAN, scientists, statisticians, and computer scientists are encouraged to contribute new ideas, enhance existing packages, and add new algorithmic techniques. These qualities make it an ideal language for the GeoChronR project.

The GeoChronR source code will be made publicly available under the GPL and source code will be made publicly available for ongoing contributions by the scientific community. The GeoChronR package will be distributed in CRAN according to common practices used by the R community for vetting and validating user contributions.

R source code is currently the #26 most popular language on Github, an advanced code management and version control system widely used for both open-source and proprietary software development projects. Under guidance from consultant Ken Collier and ThoughtWorks, GeoChronR development will conform to current best code management practices starting from the beginning of the project. As the project evolves,

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<sup>6</sup><https://wiki.lsce.ipsl.fr/pmip3/doku.php/pmip3:design:8k2:index>

periodic assurance reviews will be scheduled to ensure that code management and version control practices are effectively utilized and that the evolving project code base is well structured and easily navigable by community members.

Most researchers and users of `GeoChronR` are expected to be working on single processor commodity workstations (e.g., Windows, Linux, and OS X personal computers), making the approach highly scalable, in terms of number of users. However, this raises concerns about computational performance in this project. During the second and third years of the program, special attention will be given to boosting the performance of these tools through parallelization and multi-threaded processing. Added attention will be given to data storage and retrieval performance. ThoughtWorks' deep expertise in computational parallelization and high performance computing will be utilized to ensure that performance is acceptable, even on commodity hardware platforms.

Our software sustainability plan for `GeoChronR` is based on two principles. The first is the use of sound software engineering practices to create open software based on existing community-supported, open, and proven software. The second is an outreach plan to create a community of active users who understand and use the software for their daily work, and who will want to see the software grow. `GeoChronR` will be based partially on community-supported R packages, all of which are open source projects with a large developer community. We will coordinate our extensions with that software base and release them to the broader community.

We will set up a user forum for `GeoChronR`, and encourage users to register with their geoscience disciplines and scientific applications. This will also be a primary format for user support and updates. We will also track publications that utilize `GeoChronR`, and encourage and monitor downloads from CRAN mirrors which track usage data. These data will be the major metrics of utility and impact in the community.

## 5 Broader Impact

This project is intended to enable community-supported development of tools and contribution of well-formatted data, which this proposal only nucleates. This is intended to lower the barriers to broader use of emerging time-uncertain analysis methods in the paleogeoscience. A key challenge lies in helping the community overcome the learning curve of adopting new software. The R platform is becoming increasingly common in the community, and many paleogeoscientists have adopted the platform to take advantage of broadly useful applications on time-uncertain records. Indeed, the paper documenting the R package CLAM [Blaauw, 2010] has been cited more than 150 times since its release three years ago. To help overcome this learning curve, promote broad participation, and receive feedback on `GeoChronR`, we will host summer workshops for early-career scientists. In the 2<sup>nd</sup> and 3<sup>rd</sup> years of the program, we will hold an open application process to select 16 young scientists to travel to the campus of Northern Arizona University. These two-day workshops will train users in the basics of R and `GeoChronR`, encourage them to apply `GeoChronR` to their research projects, and when appropriate, work with participants to implement new time-uncertain analyses that will then become part of the larger toolkit. We will take advantage of these workshops to improve the usability of `GeoChronR` and develop well-articulated documentation to guide users through the package. Furthermore, to increase community participation in the project, we will broadly promote the use of `GeoChronR` at conferences and through electronic media.

A primary goal of this proposal is to recover the missing geochronologic data for many publicly archived records. For many records, differences in geochronologic methodology limits the applicability of datasets from past decades that contain valuable information to modern scientific questions. This problem will only grow worse over time, so our efforts at recovering and archiving the relevant geochronologic data will provide added value to the community, and allow for greater societal impact of previous work in the field.

This proposal will fund two early-career scientists (McKay and Emile-Geay), a graduate student at USC and two summer interns in the first and second years of the project. Through these efforts, McKay, Collier



and the student interns at NAU will contribute to the development of a geoinformatics certificate program at NAU, part of a larger environmental informatics initiative at the school.

## 6 Work plan

Acronyms: KC, Ken Collier; JEG, Julien Emile-Geay; NM, Nicholas McKay; GS, USC graduate student; SI, NAU or WDC-Paleo student interns; WDC, WDC-Paleo (see letter of collaboration).

### Year 1

- Conversion of existing Holocene databases to common, universal format and expansion with geochronological data [SI, NM, WDC]
- ThoughtWorks consulting: code management, version control, and software craftsmanship [NM, KC]
- Integration of age-modelling algorithms coded in R (CLAM, BACON) into `GeoChronR` [NM]
- Adapt age-modelling algorithms (MAFIA, BAM) from MATLAB to R [NM, JEG, GS]
- ThoughtWorks consulting: assurance of high quality design practices [NM, KC]
- Begin developing time-uncertain analysis and visualization tools, when possible, adapting from community-supported R packages [NM]
- Begin unifying the mathematical description of age-modeling algorithms [GS, JEG]
- Relay preliminary results via EarthCube RCNs and Climate Informatics [NM, JEG] (Sep 2014)

### Year 2

- Expansion of Holocene climate database with new and existing records [SI, NM, WDC]
- ThoughtWorks consulting: parallelization and high performance coding on single node commodity workstation [NM, KC]
- Develop algorithms and visualization for age-uncertain model-data intercomparison [JEG, GS]
- Finalize beta versions of analytical tools and visualizations tools [NM]
- First `GeoChronR` workshop at Northern Arizona University (August 2015), and PI coordination meeting establishing priorities for remainder of project [NM, JEG, GS]
- Limited distribution of beta version of `GeoChronR`, improving and expanding upon feedback
- Begin applying `GeoChronR` to time-uncertain climate index reconstruction in the tropical Pacific (use case 2) and analysis of the onset, duration and termination of the 8.2 ka event (use case 3) [NM, JEG, GS]
- Present results and use cases from workshop and beta distribution via EarthCube RCNs, Climate Informatics (Sep 2015), AGU (Dec 2015)

### Year 3

- ThoughtWorks consulting: R ecosystem development, conformance to open-source community standards, and review of common data structures and data science practices [NM, KC]
- Release first public version of `GeoChronR` via CRAN and WDC-Paleo
- Recruit new users via EarthCube RCNs, AGU, GSA, PAGES networks [NM, JEG, GS]
- Second `GeoChronR` workshop at Northern Arizona University (August 2016) [NM, JEG, GS]
- Present results and use cases from workshop and initial release via Climate Informatics (Sep 2016), AGU (Dec 2016)
- Continuously incorporate feedback and encourage community contributions [NM, JEG]
- Publish results of `GeoChronR`, unifying the mathematical description of age-modeling algorithms, and new science made possible by `GeoChronR` (following use cases 2 and 3)
- Public webinar introductions to `GeoChronR` led by NM [Fall 2016] and JEG [Spring 2017]

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