Age Models, Chronologies, and Databases Workshop: Complete Report and Recommendations

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SUMMARY

Paleo databases are critical cyberinfrastructure for paleoenvironmental research, especially for broad scale synoptic studies that place current environmental and climatic changes in context. Chronological control is critical for paleo studies, and chronologies and age models are essential metadata for paleo databases. Paleo databases typically comprise a large number of individual datasets acquired over a long time period. A major challenge for database managers and users is that criteria for estimating chronologies change through time rendering existing chronologies obsolete. In particular, chronologies based on calibrated radiocarbon ages become obsolete with each revision of the calibration curve, regardless of the sophistication of the age modeling technique. In addition, the sophistication of age modeling software has increased over the years. New programs, often using Bayesian techniques (Fig. 1), can now provide estimates of the uncertainties for interpolated sample ages. Most age models currently archived do not provide these uncertainties, which are nevertheless critical for assessing statistical robustness of synchronous change across multiple sites and datasets.

To address these issues, 35 scientists from 12 countries met at the Queen's University Belfast ^{14}CHRONO Centre for a three-day workshop, which was followed by a one-day software training session attended by an additional eight participants focusing on the clam (Blaauw 2010) and Bacon (Blaauw and Christen 2011) age modeling programs. The workshop was an expansion of one already planned for the Age Modeling Working Group of the Neotoma Paleoecology Database (www.neotomadb.org) and was jointly funded by PAGES and the U.S. National Science Foundation.

During the first day of the workshop, speakers discussed how various databases handle age modeling and chronology issues, calibration of radiocarbon dates, age modeling software, and database interoperability. During the following two days, breakout groups addressed the following topics: (1) Age models based on radiocarbon dating—problems caused by updates to the calibration curve; (2) Age models based on radiocarbon dating—strategies for regenerating chronologies from stored chronological data and age-model metadata; (3) Age models beyond the radiocarbon time scale; (4) Strategies for reducing the need for ad hoc age models; (5) Rankings of the quality and accuracy of dates and chronologies; and (6) Linking databases, calibration programs, and age modeling programs.

The complete recommendations are below. The most salient are: (1) Chronologies reported in the literature and stored in databases must be reproducible, and publications and databases should store sufficient data and metadata to ensure reproducibility. (2) The output from age modeling software should provide all information necessary to reproduce age models in easily storable scripts or "age model definition" files, and a common metadata standard should be developed for these files. (3) Databases should archive originally published chronologies; however, database

managers cannot be expected to reconstruct chronologies unless sufficient data and metadata are published or otherwise provided to them. (4) Because updates to the radiocarbon calibration curve and new modeling approaches may render published age models obsolete, database managers are justified in generating updated age models or storing those developed by other scientists. (5) Because ad hoc models are often difficult to reproduce, developers of age modeling software are encouraged to formally incorporate instantaneous sedimentation events, hiatuses, and sharp changes in sedimentation rate into their modeling frameworks. (6) An international open-access database for radiocarbon dates should be developed, and purchasers of radiocarbon dates should be given the option by the radiocarbon laboratories, and encouraged by funding agencies, to release their dates to it.

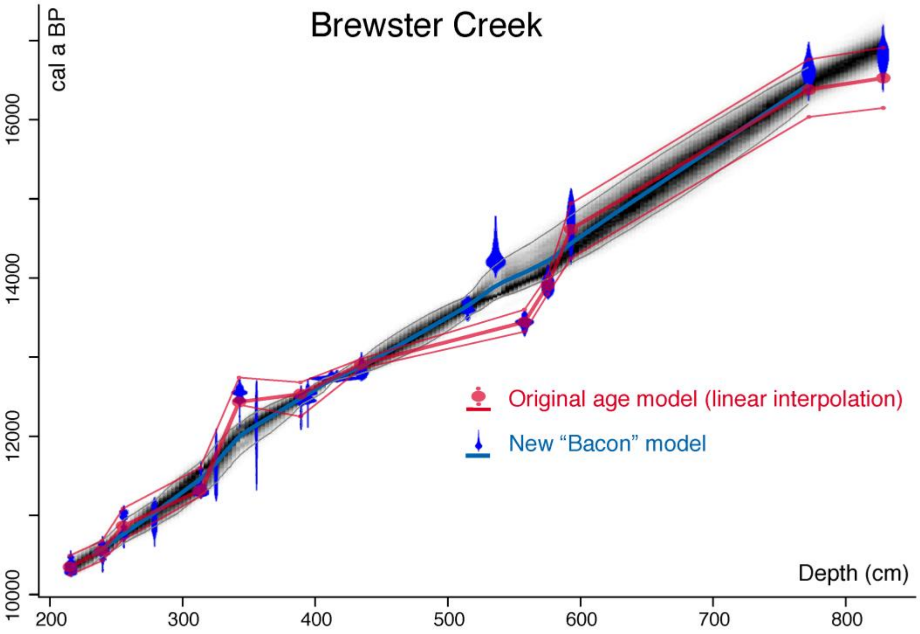

Figure 1: New Bayesian age model for the Brewster Creek site produced by the Bacon program (Blaauw and Christen 2011) overlaid with the published classical model (Curry et al 2007). The original model is based on the IntCal04 calibration curve, linear interpolation, and ad hoc rejection of reversed dates; while the Bacon model is based on the IntCal13 curve and can accommodate reversed dates, The gray-scale shading represents the relative probability within the 95% higher posterior density region (or Bayesian confidence interval). The thick magenta line is the linear interpolation between the median probabilities of the calibrated ages in the original model; the thin magenta lines connect the 95% confidence limits of the calibrated ages but are not a valid statistical representation of the confidence limits of the interpolated ages.

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SOME DEFINITIONS

Age control – an estimate of absolute age, often with a specified uncertainty, for a sample within a core or stratigraphic profile that is used to constrain an age model for that core or profile.

Age model – an algorithm used to estimate the age-depth relationship for a series of stratified paleoenvironmental data points (e.g. depths within a core or stratigraphic profile), whose relative chronological relationships are known but for which only a limited amount of absolute chronological information is available from a set of age controls. Age models are used to make estimates of ages for depths not directly associated with an age control or to resolve discrepancies among age controls. Two kinds of age models are distinguished, classical and Bayesian. Some archaeological and paleontological sequences may have age models that do not explicitly define depths, only that sections are chronologically related to other sections. An age model incorporating sample depths may thus also be called an *age-depth model*.

Classical age model – an age model in which a curve or line is fitted to a series of age-depth points with no prior assumptions about sediment accumulation rate or monotonicity of ages (Blaauw 2010). If the age controls are derived from radiocarbon determinations, they may be calibrated or uncalibrated. Any calibration is undertaken before the curve is fitted, and outliers are rejected a priori or after producing the model. Common classical algorithms include linear interpolation, linear or polynomial regression, and various splines. Many classical age models do not provide any estimate of the errors for interpolated ages, although programs such as clam (Blaauw 2010) do provide error estimates.

Bayesian age model – an age model that makes prior assumptions about sediment accumulation rates, stratigraphic superposition, and thus monotonicity of ages, and provides fully probabilistic estimates of the uncertainties in sample ages via application of Bayes' theorem. Programs that implement Bayesian age models include Bacon (Blaauw and Christen 2011), OxCal (Bronk Ramsey 2008), and BChron (Haslett and Parnell 2008). Age controls may be uncalibrated radiocarbon ages or calendar ages with uncertainties. These age models produce calibrated or calendar ages, and they can automatically deal with most cases of outlying dates.

Modern age model – an age model that provides uncertainty estimates for interpolated sample ages, regardless of whether the modeling is classical or Bayesian.

Chronology – a series of estimated ages and associated uncertainty estimates for samples in a stratigraphic sequence. Such estimates usually derive from an age model and its associated age controls.

COMPLETE RECOMMENDATIONS

1. General Recommendations

1.1. Chronologies reported in the literature and stored in databases must be reproducible, and, to ensure reproducibility, sufficient data and metadata must be provided for both the age model and its associated age controls. For geochronological measurements, these data include all the reported ages and uncertainties and associated metadata, including lab numbers and material dated. Additional metadata may be required for other kinds of age controls. The description of the age model algorithm should include sufficient information to reproduce the derived chronology, including the computer program used and any parameters or prior assumptions that were set to generate the chronology. For chronologies based on radiocarbon dates, the calibration curve used must be reported. If ages were calibrated before the chronology was generated, the calibration program and version should be reported. It is good practice to assign a version name or number to the age model used and to include this version name in all figures or analyses that rely on the age model to minimize confusion among studies employing different age models for the same data.

1.2. Currently four programs are widely used for "modern" age models that provide both interpolated ages and uncertainties of these ages: clam (Blaauw 2010), Bacon (Blaauw and Christen 2011), BChron (Haslett and Parnell 2008), and OxCal (Bronk Ramsey 2008). The program versions, metadata, and ideally scripts should be stored to enable reproduction of chronologies.

1.3. Published papers often do not provide all the data necessary to reproduce chronologies. It is recommended that producers of age modeling software provide all data necessary for reproducing chronologies in easily storable scripts or "age model definition" files. The programs should be able to read one of these files and faithfully reproduce the chronology. Although it might not be possible in all circumstances, replacement of the calibration curve in the "age model definition" file would serve to regenerate the chronology with a new calibration curve. Ideally, a common metadata standard would be developed for the "age model definition" files produced by different age modeling programs. Paleo databases should be prepared to store these files.

1.4. The lack of access to original radiocarbon data produced by the labs is a problem, especially when there are errors or omissions in published tables. Formerly, many radiocarbon labs published date lists in the journal *Radiocarbon*. However, that is no longer the case, and many, if not most, labs regard radiocarbon data as proprietary to the purchaser and will not release data to third parties, regardless of whether dates were obtained with public funding. An international open-access database for radiocarbon dates should be developed. Purchasers of radiocarbon dates should be given the option by the radiocarbon laboratories to release their dates to the database. If such a database existed, funding agencies could require that radiocarbon dates be submitted to the database and made publicly available after some suitable embargo period. Funding agencies could also require that only radiocarbon laboratories participating in the database be used. A database with standard metadata requirements could help ensure that all necessary metadata are available for published dates and help alleviate the problem of incomplete metadata reporting in published papers and associated supplemental data.

1.5. All geochronological determinations should be reported, even those dated deemed as outliers and not used for an age model, albeit with the author's explanation of why particular determinations were deemed outliers.

1.6. In general, pooling (or averaging) of radiocarbon dates is justified only when the dates are on the same object. Summing probability distributions in this context is not good practice as it has no basis in statistical theory. In the case of multiple dates obtained from individual sedimentary analysis units, rather than pooling or averaging ages, a better practice is to determine estimates of the bounding ages with uncertainties, i.e. estimates of the maximum and minimum ages of units. BCal http://bcal.sheffield.ac.uk (Buck et al. 1999) and OxCal https://c14.arch.ox.ac.uk/oxcal (Bronk Ramsey 2008) offer this capability.

1.7. Databases should include the original authors' published chronologies if the authors provide the necessary data (either in their papers or directly to the database stewards). These data include the ages with uncertainties that the authors assigned to samples, data and metadata for the age controls, parameters and priors for the age model, and a description of how the chronology was constructed. Database stewards should make a good faith effort to include published chronologies, but if the necessary age controls and other metadata or sample ages are not provided, database stewards are not obligated to attempt to reconstruct authors' chronologies, but should adopt an internally consistent approach for generating chronologies. Updates to the radiocarbon calibration curve and other advances may render published chronologies obsolete, necessitating the generation of new age models (Section 2).

1.8. Instantaneous sedimentation events (slumps, thick tephras), hiatuses, and sharp changes in sedimentation rate create difficulties for classical single-solution age models, and investigators have often created ad hoc chronologies for these situations. Chronologies from these age models are particularly challenging to reproduce. It is recommended that developers of age modeling software formally incorporate these situations into their modeling framework. Some programs already do.

1.9. Add tables/fields to Neotoma to capture information about hiatuses and instantaneous deposition events.

1.10. To simplify and aid the programmatic incorporation of calibrated radiocarbon dates in databases and applications, XML or JSON web services for calibration of radiocarbon dates would be very helpful. Services that have the imprimatur of established and published calibration programs would be especially useful, particularly in regard to recommendation 1.1.

1.11. Build Application Programming Interface (API) resources to support generation of new age models/ chronologies and for updating database chronologies. Promote semantic harmonization of these resources among different databases.

1.12. Currently, the "material dated" field in the Neotoma geochronology table is a free-text field. Convert this field to a categorical field with a lookup table. A categorical field will aid a date ranking system (see 5.3).

1.13. Establish globally unique identifiers (GUIDs) for tracking of geochronological samples and incorporate these GUIDs in paleo databases. International Geo Sample Numbers (IGSN) offer one promising example.

1.14. Organize more training workshops for use of age modeling software and paleo databases.

2. **Generation of New Age Models and Chronologies –** Neotoma and other paleo databases should incorporate or generate estimates of chronologies in the following circumstances.

    2.1. If the only existing chronology is in radiocarbon years. Calibrated or calendar year chronologies should be available for all datasets.

    2.2. If the existing chronology does not have uncertainty estimates and the chronological controls are sufficient for establishing uncertainty estimates.

    2.3. Whenever a relevant calibration curve is updated and published. Some updates do not affect the entire curve, so only chronologies with ages within the affected region(s) of the curve need be updated.

    2.4. When new chronologies are developed for a synthesis paper that utilizes the database. Major research projects that synthesize data from a large number of sites often develop new age models and chronologies, which are internally consistent, for example based on the same calibration curve.

3. **Automated Generation of New Age Models and Chronologies –** Neotoma and other databases contain hundreds or thousands of chronologies. Each of these required considerable time and effort to produce. Thus, regeneration of chronologies is challenging and automation, at least partial automation, is critical, yet must be done carefully. Age modeling programs are separate applications from Neotoma and other databases, yet to produce or reproduce chronologies for a database they must be able to acquire data from the database, and the new chronologies produced must be uploaded to the database. Essential for automating generation of chronologies from and for a database is an application programming interface (API) that enables programmatic download of data from and upload of data to the database. The Neotoma API provides for data acquisition. Neotoma also supports data upload via web services using Secure Socket Layer (SSL). Thus, the basic tools for data download/upload exist for Neotoma, although all necessary web services may not yet exist.

    3.1. For age modeling programs built in R (e.g. clam, Bacon), the “neotoma package for R” http://www.github.com/ropensci/neotoma can be further developed for acquiring data necessary for generating chronologies. An SSL module will need to be built for uploading new chronologies and associated metadata.

    3.2. As Neotoma is establishing a web service API and the neotoma package for R is built to work with this API, other paleo databases could build upon the neotoma package for R by producing semantically similar web services (see 1.11).

    3.3. In addition to chronologies developed for stratigraphic sequences, Neotoma and other databases contain records of individually dated specimens. For updating the calibrated ages of these specimens, radiocarbon calibration web services would be useful (see 1.10).

3.4. Because the construction of reliable chronologies usually requires expert knowledge of the site, stratigraphic context, and dating methods, the adoption of automated generation of chronologies should proceed carefully. Automation will work best when updates involve minor changes to existing age models, e.g. an update to the radiocarbon calibration curve.

4. **Default Chronologies –** Neotoma and other databases may provide default chronologies as a service to users who are not experts in chronological modeling. These chronologies may or may not be those originally published. Criteria for establishing the default chronology are:

4.1. Chronology is in calendar years or calibrated radiocarbon years.

4.2. If the chronology is in calibrated radiocarbon years, it is based on the most recent calibration curve.

4.3. The age model provides an uncertainty estimate for each calendar or calibrated age it outputs that is based on a sound and well documented methodology.

4.4. The age model accommodates hiatuses and instantaneous sedimentation events if they occur.

4.5. The chronology is reproducible, which depends on sufficient metadata.

4.6. The determination of default chronologies is generally the province of database managers and stewards, but should be subject to review by scientific advisory boards and representatives of the scientific community.

5. **Ranking System for Dates and Chronologies** – The accuracy with which an age model recovers the true ages of samples and quantifies the uncertainties of such estimates depends upon the quality of the age controls as well as the program. No program can overcome inaccurate, imprecise, or insufficient age controls. Database users must make judgments as to whether chronologies are adequate for their needs. Thus a ranking scheme for chronology quality could be useful. Workshop participants discussed five different ranking schemes currently in use for dates and chronologies. These vary in the criteria they use: individual dates (Blois et al. 2011), individual time horizons (Giesecke et al. 2014), or individual time series (Sundqvist et al. 2014). Because these schemes are based on somewhat different criteria, they are not mutually exclusive. Nevertheless, given this diversity, a specific scheme cannot be recommended for Neotoma or databases in general at this time. However, an automated ranking of individual dates is possible and desirable, perhaps using Blois (2011) as a starting point. Common features of samples and dating methods that can affect dating and chronology quality include the following:

5.1. The number of age controls relative to the time span of the stratigraphic sequence.

5.2. The spacing of these age controls along the sequence.

5.3. Potential for in-built age, i.e. the difference between the age of the dated material and the time of deposition or the event we actually seek to date.

5.4. Reservoir effect e.g. of dissolved inorganic carbon (“hardwater” effect) in radiocarbon samples.

5.5. Material dated, which incorporates the previous two points (see 1.12).

5.6. Laboratory treatment methods, which are particularly important for bone that is to be radiocarbon dated.

5.7. Choice of so-called “blank material” used as dating control within the dating laboratory, although this information is rarely published.

5.8. Laboratory quality control procedures and differences in the nature and scale of error among labs (not possible to rank, but laboratory lab numbers are crucial metadata).

6. Age models and chronologies beyond the radiocarbon time scale

6.1. A need exists to establish metadata standards for other geochronologic measurements besides radiocarbon, such as for OSL, argon-argon, ESR, and uranium-series dating. Whether some or all of these other methods should be stored in Neotoma or other paleo databases vs. dedicated geochronological databases needs further exploration.

6.2. There should be the capability to store floating chronologies for which sample-to-sample age differences are estimated but for which absolute ages are not known, for example interglacial varved sequences.

6.3. In a stratigraphic sequence in which some or perhaps none of the stratigraphic units may have absolute or relative age controls, the relative stratigraphic ordering of units should be stored.

6.4. Whereas absolute geochronological ages are typically associated with carefully quantified error estimates based on well documented procedures, relative ages typically are not. Examples of relative ages are event horizons, such as geomagnetic polarity reversals and transitions between marine isotope stages, or relative age units such as the Matuyama geomagnetic chron or Marine Isotope Stage 5. At present, there are no widely used methods for quantifying or recording uncertainties on relative ages. However, given the importance of uncertainty estimation in all that has gone before, this issue deserves more investment.

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Figure 2: Participants in the Age Models, Chronologies, and Databases Workshop, Queen's University Belfast ^{14}CHRONO Centre, 13-16 January 2014. *Photo credit: Peter Becker-Heidmann.*