

PaCTS 1.0: a crowdsourced reporting standard for paleoclimate data

Article

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81 Key Points:

- First version of a crowdsourced reporting standard for paleoclimate data
- The standards arose through collective discussions, both in-person and online, and via an innovative social platform
 - The standard helps meet the interoperability and reuse criteria of FAIR (Findable, Accessible, Interoperable, and Reusable).
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88 Abstract

The progress of science is tied to the standardization of measurements, instruments, and data. 89 This is especially true in the Big Data age, where analyzing large data volumes critically hinges 90 data being standardized. Accordingly, the lack of community-sanctioned data standards 91 on the in paleoclimatology has largely precluded the benefits of Big Data advances in the field. 92 Building upon recent efforts to standardize the format and terminology of paleoclimate data, this 93 94 article describes the Paleoclimate Community reporting Standard (PaCTS), a crowdsourced reporting standard for such data. PaCTS captures which information should be included when 95 reporting paleoclimate data, with the goal of maximizing the reuse value of paleoclimate 96 97 datasets, particularly for synthesis work and comparison to climate model simulations. Initiated by the LinkedEarth project, the process to elicit a reporting standard involved an international 98 workshop in 2016, various forms of digital community engagement over the next few years, and 99 grassroots working groups. Participants in this process identified important properties across 100 paleoclimate archives, in addition to the reporting of uncertainties and chronologies; they also 101 identified archive-specific properties and distinguished reporting standards for new vs. legacy 102 datasets. This work shows that at least 135 respondents overwhelmingly support a drastic 103 104 increase in the amount of metadata accompanying paleoclimate datasets. Since such goals are at 105 odds with present practices, we discuss a transparent path towards implementing or revising 106 these recommendations in the near future, using both bottom-up and top-down approaches.

107 1. Introduction

Paleoclimatology is a highly integrative discipline, often requiring the comparison of multiple
datasets and model simulations to reach fundamental insights about the climate system.
Currently, such syntheses are hampered by the time and effort required to transform the data into

a usable format for each application. This task, called "data wrangling", is estimated to consume 111 up to 80% of researcher time in some scientific fields (Dasu and Johnson, 2003), an estimate 112 commensurate with the experience of many paleoclimatologists, particularly at the early-career 113 stage. Wrangling involves not only identifying missing values or outliers in the time series, but 114 also searching multiple databases for the scattered records, contacting the original investigators 115 116 for the missing data and metadata, and organizing the data into a machine-readable format. Further, this wrangling requires an understanding of each dataset's originating field and its 117 unspoken practices, and so cannot be easily automated or outsourced to unskilled labor or 118 119 software. There is therefore an acute need for standardizing paleoclimate datasets.

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Indeed, standardization accelerates scientific progress, particularly in the era of Big Data, where 121 data should be Findable, Accessible, Interoperable, and Reusable (FAIR, Wilkinson et al., 2016). 122 Standardization is critical to efficiently query databases and analyze and plot results of analyses, 123 to remove participation barriers for new scientists or people outside the specific field by 124 explicitly describing the data rather than relying on unspoken conventions, to reduce unintended 125 errors in data management, and to ensure appropriate and complete citations for the work of the 126 original authors. While the paleoclimate community has made great strides in this direction (e.g., 127 Williams et al., 2018), much work remains. The recent adoption of the FAIR data principles 128 (Wilkinson et al., 2016) by the American Geophysical Union (Stall et al., 2017) elevates the 129 130 urgency of defining what data and metadata should be archived, and how. This article proposes a community-recommended set of preliminary reporting standards and an open platform to 131 132 determine which metadata are important for public archival, with an eye towards maximizing the 133 long-term value of hard-earned paleoclimate observations and ensuring optimal reuse.

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The need for standardization in paleoclimate research is beyond vocabulary agreement. Consider 135 the editorial of Wolff (2007), which tackled the ambiguous definition of time in the paleoclimate 136 community. The notation "before present (BP)" has become a de facto "standard" in the 137 community, although "present" means different things to different people. It is often taken as 138 Common Era (CE) 1950 (especially within the radiocarbon community), undefined, or defined as 139 some other date (e.g. CE 2000), or the year the study was performed/published. For studies 140 spanning several million years with age uncertainties in excess of 1000 years, a 50-year 141 142 difference is immaterial. However, for studies working at higher resolution (e.g. decadal to subannual), concentrating on recent millennia, this difference is consequential. Thus, an 143 agreement over the precise meaning of the term "present" turns out to be critical to many uses of 144 these datasets. The same can be said of many other metadata properties, underscoring the need 145 for common practices in paleoclimate data reporting. 146

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Given this acute need for standardization, the National Science Foundation (NSF) EarthCubefunded LinkedEarth project nucleated a discussion on data reporting practices. EarthCube (2015) defines a standard as "a public specification documenting some practice or technology that is adopted and used by a community." The emphasis on community and practice underlines the cooperative nature of standard development. If only one person uses a technical specification, it is not a standard. If it is voted on but not applied in practice, it is of little practical use.

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Standardization requires three distinct elements: (1) a standard format for the data, (2) a standard
terminology for metadata, and (3) standard guidelines for reporting paleoclimate data (i.e.,

reporting standards). We note that some prior knowledge of standardization practices (e.g., 157 which data to include) can be useful in the planning stages of data collection. As an analogy, 158 consider the organization of library cards into an old-fashioned file cabinet. For this system to 159 function, one needs (1) a set of compartments and drawers to house the information; (2) labels to 160 identify and classify the contents of the drawers; and (3) a disciplined adherence to the 161 classification system. This entails including essential information required for application and re-162 use of the cards and the information they contain. In other words, every user follows similar 163 guidelines to generate, use, and file the cards, otherwise the classification falls apart and the 164 cards may as well be stored in a random pile. 165

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This article focuses on the last requirement, namely the creation of standards for reporting paleo 167 data and metadata. It builds upon recent efforts to address the first two points. On the first point, 168 the Linked PaleoData format (LiPD, McKay and Emile-Geay, 2016) and derived vocabulary 169 agreements to describe paleoclimate data (the LinkedEarth Ontology, Emile-Geay et al., 2019) 170 provide a data container for paleoclimate data (Section 2), which is currently used in a range of 171 data analysis software (Bradley et al., 2018, Khider et al., 2018a, McKay et al, 2018). On the 172 173 second point, the National Oceanic and Atmospheric Administration (NOAA) World Data Service for Paleoclimatology (WDS-Paleo) has created a set of standard names to document 174 paleoclimate variables, the Paleoenvironmental Standard Terms (PaST) Thesaurus (National 175 176 Oceanographic and Atmospheric Administration, 2018).

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This article's aim is twofold: firstly, to provide a snapshot of the first version of the Paleoclimate Community reporTing Standard (PaCTS), as of 2019, with the understanding that this standard

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will eventually evolve; secondly, to document the process of community elicitation of such guidelines, so as to provide maximum transparency on why and how these decisions were made. We start from the premise that sampling decisions predate these reporting decisions, so the standard aims to guide an investigator's decisions as to how they should report existing measurements, e.g., at the time of publication.

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The remaining sections are organized as follows: Section 2 summarizes the relevant prior 186 standardization efforts, which serve as the foundation for PaCTS v1.0. Section 3 describes the 187 standardization process, including eliciting community feedback. Section 4 presents 188 recommendation from a group of 135 international researchers actively engaged in paleoclimate 189 research. Section 5 illustrates the application of PaCTS v1.0 to an existing paleoclimate record. 190 Finally, Section 6 concludes with a plan to disseminate the first version of PaCTS within the 191 paleoclimate community and provides a roadmap for further standards development and their 192 future applications. 193

194 **2. Background**

195 **2.1. The LinkedEarth Framework: an online approach to standard development**

The LinkedEarth project established an online platform (Gil et al., 2017) that enables the curation of metadata for publicly accessible datasets by experts and fosters the development of terminology agreements and standards for paleoclimate metadata. Our approach builds on two synergistic elements: (1) the LinkedEarth Ontology (Emile-Geay et al., 2019), which provides an unambiguous structure and terminology to describe the metadata of a paleoclimate dataset; and 201 2) the LinkedEarth Platform (Gil et al, 2017), which enables the collaborative authoring of highly-structured metadata about paleoclimate datasets using the terms in the LinkedEarthOntology.

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The LinkedEarth Ontology represents vocabulary agreements to describe paleoclimate metadata. 205 In a domain like paleoclimatology, we usually can distinguish the different kinds of objects that 206 207 we want to describe (i.e., a sample, a measurement, a dataset, etc...) and the relationships used to describe those objects (e.g., a measurement is taken from a sample and therefore they are related, 208 the measurement in is a dataset and therefore they are related, etc...). An ontology is a formal 209 210 way to represent objects and their properties, and they represent consensual knowledge that helps a community describe major concepts in the domain using common terms. Specifically, an 211 ontology formalism allows the representation of objects types as "classes", and relationships as 212 "properties" of those classes. Classes can have subclasses, and a given class can be a subclass of 213 several classes. For example, the class "proxy archive" can have "coral" as a subclass, and the 214 class "repository item" can have "sample" as a subclass". A feature of ontologies is that they 215 allow the creation of machine-readable metadata, i.e., data descriptions that can be queried 216 programmatically by machines to retrieve datasets of interest. Thanks to the ontology, machines 217 can navigate through metadata and discover data that otherwise would be hidden to them. 218 LinkedEarth relies on semantic web technologies to represent ontologies, specifically the Web 219 Ontology Language (OWL) standard of the World Wide Web Consortium (W3C) (W3C OWL 220 221 Working Group, 2012). More details are provided in Emile-Geay et al. (2019).

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The LinkedEarth Platform allows users to 1) describe paleoclimate datasets using the terms available in the LinkedEarth Ontology, and 2) propose new terms if they cannot find an

appropriate one in the ontology. The LinkedEarth Platform is a sociotechnical system, and as 225 such it provides technology infrastructure coupled with social processes that support terminology 226 and standards convergence. When users describe a paleoclimate dataset, the terms in the existing 227 LinkedEarth Ontology are offered to them as editable forms and completion commands, which 228 promotes adoption. If a user does not find a term that is appropriate for their dataset, they can 229 230 create a new term on the fly. Such new terms can then be discussed on the platform, building community consensus on their definitions and the essential status of their inclusion to a dataset. 231 The social extensions of the LinkedEarth Platform allow working groups to organize activities 232 by users with similar expertise to build a common vocabulary. Each working group was assigned 233 a special page on the LinkedEarth Platform to nucleate their activities, including discussions and 234 polls for rapid community feedback. The terms discussed within these working groups form the 235 crowdsourced part of the LinkedEarth Ontology. The social editorial processes eventually will 236 lead to a new version of the LinkedEarth Ontology. The LinkedEarth Platform and its associated 237 social processes are described in detail in Gil et al. (2017). 238

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The LinkedEarth Platform is implemented as an extension of the Semantic MediaWiki 240 framework (Krötzsch and Vrandečić, 2011), Semantic wikis augment traditional wikis with the 241 ability to structure information through: 1) semantic annotations, which enable the assignment of 242 a class (or category) to an object in a wiki page, and properties (or qualifiers) that are useful to 243 244 describe that object; and 2) automated reasoning capabilities that exploit those annotations to organize the wiki's knowledge (Gil, 2013). For example, if the page for "Los Angeles" is 245 annotated as being in the class "city" and having a property "location=California", and the page 246 247 for "California" has a property that "location=US" then the semantic wiki can infer that Los

Angeles is in the US even though that was not explicitly stated. Semantic wiki pages can also 248 include queries that are executed when the page is visited, so dynamic content is created in a way 249 that is up to date with the latest additions. Semantic wikis also have facilities to track edits 250 together with the data and contributor, so that the provenance of edits can be examined and 251 undesirable ones can be easily undone. The content of semantic wikis becomes part of the open 252 Semantic Web, as it can be published as a set of linked Web objects in the Web of Data, 253 following Linked Data Principles (Heath and Bizer 2011). With this approach, the metadata for 254 all paleoclimate datasets defined in the wiki becomes openly available on the Web, machine 255 readable, and can be queried programmatically by any application. More details are provided in 256 Gil et al. (2017). 257

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2.2. Previous and concurrent efforts towards a data standard

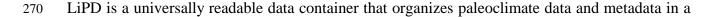
The discussion below is non-exhaustive and only focuses on the relevant efforts that have 259 sparked the discussion about PaCTS. 260

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2.1.1. Origins of a standard format for paleoclimate data

Climate modeling has greatly benefitted from the netCDF data format (Unidata, 2019), designed 262 to support the creation, access, and sharing of array-oriented data, including climate model 263 output. Despite the importance of paleoclimate data availability for model evaluation (Masson-264 Delmotte et al, 2013), until recently there was no universal container to describe, store, and share 265 these datasets. Emile-Geay & Eshleman (2013) first introduced the idea of a flexible container, 266 where metadata would be stored semantically with the numeric data in tabular form. This 267 concept was the basis for the Linked Paleo Data (LiPD) format (McKay and Emile-Geay, 2016). 268

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uniform way. It is based on JSON-LD (JavaScript Object Notation for Linked Data), a JSON-271 based format compliant with the Linked Data paradigm. JSON is a lightweight data interchange 272 format that is easy for humans and machines alike to read and write. LiPD has six distinct 273 components: root metadata (e.g., dataset name, investigator, version); geographic metadata (e.g., 274 coordinates, descriptive location such as a country or city); publication metadata (e.g., authors, 275 title, journal, DOI); funding metadata (e.g., funding agency and grant number); PaleoData, which 276 includes all the measured (e.g., Mg/Ca) and inferred (e.g., sea surface temperature) 277 paleoenvironmental data; and ChronData, which mirrors PaleoData for information pertaining to 278 279 age. These components provide the rigidity necessary to write robust codes around the format, while remaining extensible enough to capture (meta)data as rich as the users want to provide for 280 them. Utilities in Matlab, Python, and R (Heiser et al., 2018) allow users to interact with the files 281 (specifically, to read, write, query, or filter datasets matching specified conditions). 282

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In many ways, LiPD is intended to be the netCDF of paleoclimate observational data. However, 284 although both LiPD and the LinkedEarth Ontology provide a standard way to describe a 285 paleoclimate dataset, they say little about what information should be stored to ensure re-use. 286 The endorsement of netCDF by a broad community further benefited from the adoption of the 287 Climate and Forecast (CF) conventions (Gregory, 2003). The CF conventions define metadata 288 describing what the data in each variable represents, and the spatial and temporal properties of 289 290 the data. In other words, it defines both a set of common terms (a standard vocabulary) and a reporting standard. Efforts toward standardization of common terms have been undertaken by 291 WDS-Paleo in the form of the PaST thesaurus (National Oceanographic and Atmospheric 292 293 Administration, 2018), which provides the preferred option for a standardized name and

definition. PaCTS details a crowdsourced approach for deciding what information should be included when reporting paleoclimate data, a "CF convention" for paleoclimate datasets.

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2.1.2. Archive-focused initiatives

Attempts at paleoclimate data standardization have a long history. For datasets derived from 297 298 wood archives, LinkedEarth relied on the tree-ring data standard, TRiDaS (Jansma et al., 2010), which complies with established data standards such as Dublin Core (DCMI Usage Board, 299 2008). The TRiDaS project aimed at defining the properties that are used in the dendro 300 community and give them a consistent name (i.e., a controlled vocabulary) and identifying 301 whether the quantity should be mandatory and repeatable (i.e., best practices). These efforts help 302 inform the PaCTS one for wood archives, though it should be noted that tree-ring science is far 303 304 broader than dendroclimatology, involving applications to paleofire, landscape evolution, paleoecology, art history, and archeology. Because PaCTS is focused on paleoclimate, we re-305 used the relevant subset of the TRiDaS standard. 306

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A discussion regarding paleoceanographic data standards was started during the Paleoclimate 308 Model Intercomparison Project (PMIP) Ocean Workshop 2013 - Understanding Changes Since 309 the Last Glacial Maximum (hereafter, PMIP LGM) in Corvallis, Oregon in December 2013. 310 311 Given the expertise of the working group members, the discussion focused on marine sedimentary archives and was summarized into a document, which is available on the 312 LinkedEarth Platform (Kucera et al., 2013). Their recommendations served as the foundation for 313 a preliminary reporting standard for records based on marine sedimentary archives. Although the 314 group identified recommended properties to be included with marine datasets, they did not 315 propose a complete vocabulary nor a subset of required properties for acceptance in a database. 316

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The Marine Annually Resolved Proxy Archives (MARPA) working group, nucleated under the 318 EarthCube umbrella, is one of the first grassroots efforts within the paleoclimate community to 319 enhance and facilitate the archiving and sharing of paleoclimate data as they pertain to annually 320 resolved archives (e.g., corals, mollusks, coralline algae, and sclerosponges; Dassié et al., 2017). 321 Their efforts included a registry of physical samples as well as their associated geochemical data 322 and metadata, which are our primary focus here. The MARPA group summarized their 323 recommendations in a document that was circulated among the community and constitutes the 324 backbone of the recommendations presented here. Most of these recommendations were also 325 applicable to other archives, rather than MARPA-specific, underscoring that despite their 326 diversity, paleoclimate datasets retain common core properties that facilitate multi-proxy 327 syntheses and comparisons. 328

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The Speleothem Isotopes Synthesis and Analysis (SISAL) group was formed under the 330 international Past Global Changes (PAGES) project and aimed at bringing together speleothem 331 scientists, process modelers, statisticians, and climate modelers to develop a global synthesis of 332 333 speleothem isotopes that can be used to further our understanding of past climate variability and in model evaluation. As part of this initiative, a template was created, outlining the necessary 334 metadata for speleothem-based records (Atsawawaranunt et al., 2018). This template (Comas-335 336 Bru & Harrison, 2019) forms the backbone of properties applicable to speleothems-based records presented here. 337

338

2.3. Workshop on paleoclimate data standards

339 The workshop on paleoclimate data standards held in Boulder, USA in June 2016 (Emile-Geay

& McKay, 2016, Figure 1) served as a focal point to initiate a broader process of community 340 engagement and feedback solicitation, with the goal of generating a community-vetted standard 341 for reporting paleoclimate data. Workshop participants identified the necessity to distinguish a 342 set of essential, recommended, and desired properties for each dataset. By default, any and all 343 information was considered *desired*, though we shall see exceptions to this principle. A subset of 344 the archived information should be recommended to ensure optimal reuse of the dataset. Yet a 345 smaller subset of this information is defined as *essential*, meaning that the dataset cannot be 346 reused reliably or at all without these critical pieces of information. 347

348

A consensus emerged that these distinctions are archive-specific; for instance, what is needed to 349 meaningfully reuse MARPA records could be quite different from what is needed to 350 meaningfully reuse an ice core dataset. It was therefore decided that experts on particular 351 paleoclimate archives organized into working groups (WGs) would be best positioned to 352 elaborate and discuss the components of a data standard for their specific sub-field of 353 paleoclimatology. Consequently, seven WGs were created on the LinkedEarth Platform centered 354 around the main archives used in paleoclimate studies: historical documents, ice cores, lake 355 356 sediments, marine sediments, MARPA, speleothems, and tree rings. A call for additional WGs was made in the fall of 2016. Observations common to two or more archives (e.g., alkenones) 357 were discussed in one WG with a link to the discussion in other WGs. It is also critical to ensure 358 359 interoperability among standards to enable investigations using multiple observations on the same archive as well as across archives; to that end, three longitudinal WGs were created to deal 360 361 with information common to all archives (such as publication, geographical coordinates, funding 362 information), to report uncertainties in the record, and to report how chronologies were

363 established.

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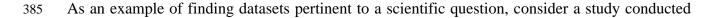
The workshop participants also identified the need to have a separate set of requirements for newly generated datasets and legacy datasets, for which less metadata would likely be available. In PaCTS v1.0, a legacy dataset is defined as a dataset that is not being archived by the author(s) of the original study.

369 3. Towards PaCTS

370 **3.1. Working groups**

Rules of engagement on the LinkedEarth Platform were published in the fall of 2016 along with 371 the establishment of seven WGs (ice cores, lake sediments, marine sediments, MARPA, 372 373 speleothems, trees, and uncertainties, Figure 1). Three WGs (chronologies, cross-archive, and historical documents) followed in the spring of 2017 as additional archives and common 374 information to all archives were identified. Each WG leader was tasked to organize their 375 376 subcommunity either directly on the platform, through videoconferences, meetings at conferences, and/or other working groups (e.g., MARPA group and the PAGES SISAL group). 377 The WG leaders were tasked to regularly update the discussion directly on the LinkedEarth 378 platform or provide a document for integration on the platform. One difficulty in defining 379 380 desired, essential, and recommended properties was related to the expected use of the data: depending on what one wants to do with the data, one needs different metadata. By far, the most 381 important and metadata-hungry task is to perform queries to find datasets pertinent to a scientific 382 question. 383

384



by a paleoceanographer who wants to characterize millennial-scale sea surface temperature 386 (SST) variability during the Holocene epoch (Khider et al, 2016). In the current research 387 ecosystem, a typical workflow would consist of querying several databases to find suitable 388 records, extract the data, consult the original publication(s) for additional metadata (e.g. author's 389 definition of 'present'), reformat the data into a coherent format for analysis, apply spectral 390 analysis to examine the frequency content of the records, perform some statistical analysis of the 391 results, and visualize them. In an ideal world, the query, preferably from a single database, 392 should (1) find records that span the Holocene, (2) find the subset of those that primarily reflect 393 394 SST, and (3) find the subset of that subset with a specified resolution (e.g., finer than 200 years) to have at least five data points per 1,000-year cycle (a permissive assumption for this sort of 395 work). Simple though it may seem, this query requires the following (meta)data: (1) a measure of 396 age (time) and minimum and maximum values of the time series; (2) an estimate of SST, as an 397 inferred variable, and/or Mg/Ca, U^{k'}₃₇, TEX₈₆, or microfossil assemblages as measured variables 398 from which SST can be inferred; and (3) temporal resolution, calculated from the data. 399

400

Other types of basic queries include: searching for a particular publication, using either the
digital object identifier (DOI), title, journal, or authors; and searching by the type of archives.
Defining the search parameters for these complex queries on the LinkedEarth platform (Khider
& Garijo, 2018) sparked the discussion for the needed properties.

405

A standard helps not only with the menial task of searching for records in a database. Such a standard can also assist with doing the science *per se*, by ensuring that the required information is present in the dataset. For instance, making a simple map of all the records in a database by archive types (Figure 1a of PAGES 2k Consortium, 2017) requires each dataset to report latitude,
longitude, and the archive type. More complex data analysis requires more information: to
investigate the effect of age uncertainties (e.g. with the Bchron (Haslett and Parnell, 2008) or
BACON (Blaauw and Christen, 2011) packages), or to establish new depth-age models (Blois et
al., 2011; Giesecke et al., 2014), one needs the raw radiocarbon measurements, their
measurement uncertainties, and associated depth in the archive.

415

3.2. Community surveys

To decide which of the properties identified within the various WGs should be considered 416 essential, recommended, or desired, we first gathered input via the LinkedEarth platform (Figure 417 2a). As of August 1st 2018, it was home to 207 polls, with 796 votes given by 32 different users. 418 419 On average, each question received 3 votes, with some questions receiving no votes and others as many as 27. Note that some questions were duplicated across different WGs and the final 420 count presented here takes into account all votes received on the platform. The low number of 421 422 votes can be partially attributed to the fact that voting was only possible after authentication onto 423 the platform, creating a barrier to widespread participation. To broaden community involvement, the polls were then threaded on Twitter from the LinkedEarth account with voting allowed over a 424 seven-day period (Figure 2b). The Twitter polls increased engagement (by a factor of 3 on 425 426 average), and also led to discussions that were then moved to the LinkedEarth platform for traceability of decisions. 427

428

Finally, by request from the community, the questions were summarized in a survey distributed to the paleoclimate community through the ISOGEOCHEM, CLIMLIST, paleoclimate and cryolist list-servs as well as the PAGES e-news, website, and social media. The survey contained

603 questions across all working groups for which respondents were asked to determine whether 432 each property is deemed essential, recommended, or desired for new and legacy datasets, in 433 addition to open-ended questions and prompts for community feedback. The survey was more 434 comprehensive than the polls on the LinkedEarth platform or Twitter since all questions were 435 framed to allow for a response for legacy and new datasets. On the other hand, the LinkedEarth 436 platform also contains duplicate questions across various WGs (e.g., "should depth be reported 437 as essential, recommended, desired), polls aiming to define the scope of the datasets housed on 438 LinkedEarth (e.g., "should the LinkedEarth platform only contain datasets that appear in peer-439 reviewed publications?"), and the operating definition of legacy versus new datasets that was 440 then used in the survey. Ninety-five scientists participated in the survey. Each question on the 441 survey received on average 54 answers. 442

443

Paleoclimatology is a multi-disciplinary effort where researchers typically have expertise in one 444 or more proxy systems (e.g., different observations on the same archive, similar observations on 445 different archives, or a mix of different sensors, observations and archives). Scientists are often 446 led to compare their own datasets to others obtained from proxy systems with which they are less 447 448 familiar. Consequently, the metadata they need tend to differ based on their level of expertise (it is easier to "fill in the blanks" in one's own area of expertise). For instance, an ice core expert 449 interested in comparing their deuterium record with a nearby record of SST would most likely 450 451 only require the age at each horizon and associated SST. On the other hand, an expert on foraminiferal Mg/Ca-based SST reconstruction may also need information about the cleaning 452 methodology or the number of individual foraminifera in the sample. To ensure that both needs 453 454 were represented, respondents were encouraged to complete the entire survey, rather than focus

455 exclusively on their own areas of expertise.

456 **3.3. Survey responses**

The 95 survey responses were then combined with the Twitter and LinkedEarth platform poll 457 answers (Figures 3, 4 and Supplementary Information). In total, 135 participants from North 458 America (52%), Europe (36%), Australia (5%), Asia (4%), South America (2%) and Africa (1%) 459 were identified across the survey and LinkedEarth platform. Since voting on Twitter is 460 anonymous, it is impossible to identify these voters or establish whether they voted on other 461 462 platforms. We are aware that some researchers may have answered the same question several times on the various platforms. Since the number of survey answers dwarfs the number of votes 463 on Twitter and the LinkedEarth platform (Supplementary Information) and Twitter does not 464 465 track the user names associated with the votes, we did not attempt to correct for multiple responses. Therefore, 135 contributors represent our best estimate for the number of total 466 participants. 467

468

Most of the polls on Twitter and the LinkedEarth platform referenced legacy versus new datasets. However, in the cases where the dataset status was not specified, we assumed that the question referred to a new dataset only. Furthermore, if a question was repeated on various WGs (e.g., latitude, longitude), the number of votes were tallied and included in the total count for the cross-archive metadata reporting (see Section 4.1). Responses on the survey, Twitter, and the LinkedEarth platform were given equal weight.

475

For each of the properties, we identified respondents' recommendation for both new and legacy datasets as the majority vote. We used mind maps to visually organize the hierarchical

information, keeping the relationship intact (Figures 5) and mosaic plots to display the 478 frequencies of the essential, recommended, and desired categories for each working group 479 (Figure 6). Overall, the community identified 208 properties (69% of polled properties) as 480 essential, 82 (27%) properties as recommended, and 12 (4%) as desired for new datasets. For 481 legacy datasets, fewer properties were deemed essential: 131 (44%) of polled properties versus 482 136 properties (45%) were considered recommended and 34 properties (11%) were identified as 483 desired. This difference is not unexpected and highlights the fact that legacy datasets, although 484 not as metadata-rich as new datasets, are still valuable to the community (Figure 6). 485

4. PaCTS v1.0: Paleoclimate Community reporting Standard 486

This section is based on the recommendations made in the various WGs, which were then subject 487 488 to polling through the LinkedEarth platform, Twitter, and the survey. We are aware that these recommendations may be incomplete for some archives, a point discussed in Section 6. A list of 489 these properties, definitions, and associated recommendations are available on the LinkedEarth 490 491 platform.

- 492

4.1. Cross-Archive Metadata

Despite their diversity, paleoclimate records (and compilations thereof) share common metadata 493 properties such as contributors, geographical information (e.g., coordinates, site name), 494 publication information (e.g. authors, title, journal, DOI), funding information, and general 495 information about the paleoenvironmental and chronology data (e.g., "should the raw data be 496 included?"). In total, the community identified 54 properties applicable to all archives (Figures 5 497 and 7). 498

499

For new datasets, 36 of these properties were identified as essential, 9 as recommended and 9 as 500 desired. It is not surprising that 67% of the properties were voted as essential since these 501 properties are critical for the data reuse with no expert knowledge about the proxy systems or 502 paleoclimate. Likewise, 24 of these properties (44%) were identified as essential for legacy 503 datasets. For a dataset to be reused, information regarding the location, publication, and 504 interpreted chronology and paleoenvironmental variables is critical. Hence, several researchers 505 commented that new datasets should contain both the raw and interpreted data. The bar for 506 legacy datasets should be lower, recognizing that much of the desired data may no longer be 507 available, and that interpreted data are still useful for many applications. 508

509

In addition to the properties identified, a dataset DOI and a dataset license would also promote data reuse. LinkedEarth is not setup to mint DOIs directly but they can be obtained through other platforms such as PANGAEA, Dryad, or FigShare. The registry of research data repositories, re3data, gives information on whether a repository provides persistent identifiers. The Creative Commons (CC-BY) license is recommended for paleoclimate data since under this license, other researchers are free to share and adapt materials while giving appropriate credit to the original contributor of the resource.

- 517 **4.2.** Archive-specific metadata
- **5**18 **4**.

4.2.1. Ice cores

The ice core WG identified 16 properties specific to glacier ice, including information pertaining to the archive, such as melt in transport, storage conditions, the observations available for the archive, and the chronology. For new datasets, eight properties were deemed essential and eight

- recommended. The number of essential properties dropped to four for legacy datasets with threeproperties deemed recommended (Figures 5, 6 and 8).
- 524

As with historical documents, most survey respondents were not experts on records generated on ice cores and therefore only responded for properties they were likely to use.

527

4.2.2. Lake Sediments

The lake sediments WG reported 54 properties specific to this archive, which were grouped by proxy sensor/observation types: particle size, mineralogy, imagery data, accumulation rate, and compound specific isotopes. Whereas some properties were common across the various types of observations (i.e., units, interpretation, pre-treatment methods), many were observation-specific (e.g., source of compound for compound-specific isotopes), highlighting the necessity of detailed sets of guidelines down to the proxy observation level to meet researchers' needs.

534

535 For new datasets, 39 properties were identified as essential and 15 as recommended. For legacy datasets, 25 were seen as essential, 28 as recommended, and 1 as desired (Figures 5, 6, and 9). In 536 addition to these 54 properties, the WG started a discussion on how to best report the concept of 537 depth in the archive. Although several WGs identified depth (i.e., position in the archive sample) 538 539 as an essential property, especially for new datasets, none had defined how this depth should be reported. The majority of the respondents indicated a preference to report top and bottom depth 540 for both new and legacy datasets although several respondents proposed to lower the bar for 541 legacy datasets to whatever is available for these records. 542

543

Respondents also noted that pictures of the core after the sampling process would be useful. Whether these pictures should be available with the data or stored in the database of the physical sample repository is a decision best left to individual researchers, based on their constraints and mandates by funding entities.

548

4.2.3. Marine sediments

The marine sediments WG identified 48 properties specific to this type of archives. These 549 properties were divided into 6 groups, according to the type of observation: general sampling, 550 bulk sediment geochemistry, foraminifera geochemistry, alkenones, the glycerol dialkyl glycerol 551 tetraether (GDGT) proxies, and micropaleontology. The foraminifera geochemistry category was 552 further subdivided into stable isotopes, boron isotopes, and trace elements. Although some of the 553 554 requirements were common to all observations, this WG included several observation-specific properties such as the cleaning methodology for foraminiferal trace elements or raw peak areas 555 for GDGTs. 556

557

558 For new datasets, 36 properties were identified as essential and 12 as recommended. The number 559 of essential properties drops to 24 for legacy datasets, with the remainder considered 560 recommended (Figures 5, 6 and 10).

561

4.2.4. Coral, mollusks, and other annually resolved marine records

The properties for these archives were taken from the spreadsheet the MARPA group had circulated online for feedback. Most of these properties were applicable to all archives reporting geochemical properties and were therefore incorporated into the cross-archive WG and questions. Two archive-specific properties were also identified: interpolated chronologies (i.e., distance from core top translated to time usually a calendar day for each sample then interpolated

567 t	to even monthly intervals) and X-ray pictures (and associated drilling path). For both new and
568 l	legacy datasets, the raw (distance from core top), interpolated chronologies, and X-ray pictures
569 V	were considered essential and recommended, respectively (Figure 5 and 6). The reporting of
570 g	growth increments in mollusks and corals is still an ongoing discussion within MARPA.

571

4.2.5. Speleothems

When constructing their database (Atsawawaranunt et al., 2018), the SISAL WG identified 23 properties specific to speleothem records. The SISAL database only focuses on stable isotopes in speleothems and these properties only apply to this proxy system. These properties can be further subdivided into four categories describing the cave and modern cave conditions, the physical sample, and information about the sample data. For new datasets, 11 properties were considered essential and 12 recommended. For legacy datasets, only 2 properties were considered essential and 21 were marked as recommended (Figures 5, 6 and 11).

579

Although "evidence for equilibrium" (e.g., the Hendy test; Hendy, 1971, or monitoring data that supports equilibrium precipitation of calcite) was narrowly voted as essential for new datasets and recommended for legacy datasets, three respondents (two on Twitter and one on the survey) expressed concerns about the value of this property as it "rarely shows up in monitoring data" and the Hendy test has been "abused" by the paleoclimate community. This illustrates the need for an evolving standard, one that fits the needs of the community and changes as our scientific understanding about proxy systems increases.

587

4.2.6. Tree-based records

The tree ring community has a long history of developing and adopting data standards; however, the metadata capacity or requirements in earlier data formats (e.g., Tucson, Heidelberg, Sheffield, CATRAS and Belfast amongst many others) were limited by the technology of the decade in which they were created (Brewer et al. 2011). The 35 properties in the survey were taken from TRiDaS (Jansma et al., 2010) and from the proposed tree-ring isotope databank (Csank, 2009). TRiDaS was chosen as a starting point as it was designed as a standard to represent dendrochronological data across its many subdisciplines, including dendroclimatology. TRiDaS therefore includes many (optional) properties as essential or recommended that are not applicable to datasets collected for paleoclimate reconstructions.

597

For new datasets, 26 properties were considered essential, 7 recommended, and 2 desired. For 598 legacy datasets, 19 properties were voted on as essential, 9 as recommended, and 7 as desired 599 (Figures 5, 6, and 12). Several researchers were confused about the terms used in TRiDaS, 600 suggesting that the standard may be too broad for most paleoclimate applications and should be 601 further refined if it is to be widely adopted. The reason for this confusion may be because 602 TRiDaS was initiated by the cultural dendrochronology community (e.g., dendroarcheology, art 603 and building history) in a response to the more pressing need for standardized metadata in these 604 disciplines. Despite attempts to engage all subdisciplines of dendrochronology in the 605 606 development of TRiDaS, the cultural aspects of the standard were more fully implemented due to the greater participation of users from these areas of research. 607

608

Nevertheless, a subset of the fields defined in TRiDaS were used as a starting point for discussion for PaCTS v1.0. Many fields within TRiDaS are already addressed in the crossarchive metadata and were disregarded, leaving only dendro-specific fields. These were then supplemented by fields for tree-ring isotope data taken from the tree-ring isotope databank

proposed by Csank (2009). Regretfully, discussion of the suitability of these fields among the 613 dendroclimatology community has been limited and the list of initial fields was not subsequently 614 refined. The public voting process has resulted in a number of fields being marked as 'essential' 615 that are not routinely (if ever) collected for dendroclimatological research. Furthermore, some of 616 the quantities that are being proposed are difficult to measure or know, raising the issue of 617 whether these properties are even desired. Some of the properties are a characteristic of the data 618 themselves ('ring count') and not metadata per se. These may be useful as convenience fields 619 when querying large data collections (rather than having to extract and calculate). 620

621

The confusion in the voting process could reflect confusion over whether PaCTS v1.0 is to be a data standard applicable to all dendrochronological datasets or exclusively to those collected for use in climate reconstructions, for which a smaller number of 'essential' fields would be required. It could also reflect sampling bias in the voting process related to the composition of the WG.

627

While the work described here is clearly an important step towards incorporating dendroclimatological data into a universally applicable paleoclimate data standard, there remains a great deal of work to be done. This work needs to begin with discussions that engage a much broader cross-section of the dendroclimatological community and refined criteria in subsequent surveys.

633

4.2.7. Documentary archives

Historical documents differ quite significantly from the other archive types presented in PaCTS
v1.0. Documentary data are extracted from written sources (books, chronicles, newspaper, etc)

and each of these sources in the dataset needs a reference to the publication metadata (in addition 636 to the scientific publication of the data in a journal). The raw data most comparable to 637 measurements on other archives are quotes, i.e., text strings in any language cited from the 638 source from which location, time, and event are extracted. Every single data point in the set can 639 thereby have a different location and a variety of parameters describing the event (Glaser, 1996). 640 The time step can be, but is not necessarily, periodic. The quote might contain information 641 regarding the temperature in a city, precipitation conditions, and the resulting water level in a 642 river, as well as statements concerning harvest amount and quality of a certain crop. The 643 resulting data type can be boolean (for presence/absence), integer (for indices), real numbers 644 with units for measurements, or enumerations (Riemann et al., 2016). 645

646

The documentary archives WG identified nine properties which concerned the source material, 647 including original scans of the documents, quote ID, language, and reference to the source 648 material (e.g., DOI, license, page). Among these nine archive-specific properties, four (the quote, 649 reference to the quote, the quote ID and the quote's DOI) were voted as essential and five as 650 recommended for new datasets. For legacy datasets, only two (the quote and its reference) were 651 identified as essential (Figures 5, 6 and 13). Four survey respondents indicated that they were 652 least familiar with this type of archive, which may help explain why fewer properties compared 653 to other archives were considered essential for optimal reuse of the resource by researchers not 654 655 familiar with the intrinsic details of the archive.

656

4.3. Uncertainties

657 The Uncertainties WG identified seven properties applicable to most records. These properties658 fell into two broad categories concerning the uncertainty in the measured variable (analytical

uncertainty, number of repeat measurements, and reproducibility) and the uncertainty associated 659 with models to infer variables, including chronologies (output statistics, output ensembles along 660 with the parameters and the publication in which the model is described). For new datasets, four 661 properties (analytical uncertainty, number of repeat measurements, the publication and 662 parameters of the model) were deemed essential and the other three recommended. For legacy 663 datasets, only one was deemed essential (number of repeat measurements) while the rest were 664 recommended. This highlights the commitment of the community to better characterize 665 uncertainties in paleoclimate records and the acknowledgement that uncertainty has often been 666 ignored when reporting datasets in the past, making it difficult to include metadata for legacy 667 datasets (Figures 5, 6, and 14). 668

669

Respondents voted on reporting the analytical uncertainty and reproducibility as "2-sigma" (estimated as the standard error of the mean), although a point was raised that the reporting should be community-specific, following their own accepted standards (e.g., radiocarbon, Stuiver et al., 1977, Millard et al., 2014), but clearly indicated in the metadata. A compromise is to keep community-specific standards while encouraging 2-sigma reporting if there is no preexisting standard.

676

For models, the method used should be documented both in the papers and with the data, with publication information about the software and parameters used being considered essential for new datasets. For legacy datasets, all information about the model is considered recommended.

680

Confidential manuscript submitted to Paleoceanography and Paleoclimatology

The Uncertainties WG has barely scratched the surface of uncertainty reporting in paleoclimate 681 studies. Although several other WGs have reported that uncertainty should be an essential 682 parameter, there is not yet a clear path forward as to how this uncertainty should be 683 unambiguously reported. However, there is some consensus that the method of reporting does 684 not matter as long as the method is clearly described. To do so, the LinkedEarth Ontology 685 (Emile-Geay et al., 2019) offers several paths forward. The class "Uncertainty" can refer to a 686 single value for all the data values, to a list of values of equal length as the uncertain variable, 687 and to models output stored in ensemble, summary, and distribution tables. 688

689

Consider the example of radiocarbon dating. Each radiocarbon value is associated with an 690 uncertainty that is often reported in a separate column of the measurement table. This 691 radiocarbon-age uncertainty is then translated (via a calibration curve) into a calendar age 692 uncertainty that is also stored in a separate column. In both of these cases, the uncertainty is a 693 variable that can be described with the same richness as other columns in the data table. 694 Furthermore, probabilistic age modeling software such as Bchron (Haslett and Parnell, 2008) and 695 BACON (Blaauw et al., 2011) for radiocarbon, HMM-Match (Lin et al., 2014) for stratigraphic 696 697 alignments, and the Banded Age Model (Comboul et al., 2014) return possible age distributions around the calendar age value as well as age model ensembles for each depth in the paleorecord. 698 In this particular example, each measured value has at least one associated uncertainty value, 699 700 possibly an entire probability distribution.

701

On the other hand, uncertainty associated with measurements of trace elements and stable isotopes is often reported as the uncertainty of the standard or a handful of replicates that are taken to represent the uncertainty for all values. The LinkedEarth Ontology (Emile-Geay et al.,
2019) allows for the specification of not only the values and units of the uncertainty, but also
how this uncertainty is estimated and the level at which it is being reported (e.g., one standard
error of the mean).

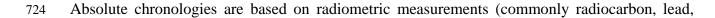
708 **4.4. Chronologies**

The Chronologies WG identified 54 properties, 43 of which were deemed essential for new datasets, 10 recommended and 1 desired. For legacy datasets, 30 were identified as essential, 22 as recommended, and 2 as desired (Figures 5, 6 and 15).

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713 Chronologies are obtained using two methods: absolute and relative. Relative chronologies often 714 involve the alignment of one paleoclimate time series with another of known age. For instance, benthic foraminifera stable oxygen isotope (δ^{18} O) records have often been aligned to the dated 715 LR04 benthic δ^{18} O stack (Lisiecki and Raymo, 2005). For this type of chronology, the original 716 measurements (e.g., benthic foraminifera δ^{18} O), the alignment target (e.g., LR04 benthic δ^{18} O 717 stack), its associated reference chronology (e.g., LR04 age model) and alignment method (e.g., 718 719 HMM-Match (Lin et al., 2014)) should be clearly identified (essential) for both new and legacy datasets. We acknowledge that there is potentially more work to be done to devise a standard for 720 relative chronologies, which should include an integration framework for biostratigraphy, 721 paleomagnetism, stable isotopes chronologies, and orbitally-tuned chronologies. 722

723



and uranium-decay series, or terrestrial cosmogenic nuclide), layer-counting, counting of annual cycles in geochemical/isotopic proxies, dendro- or tephrochronological crossdating, or luminescence. In addition, some records are characterized by floating chronologies that are absolutely dated (within the uncertainty of the radiometrically derived age), but which have a precise internal chronology due to clear annual banding/cycles (e.g., U-series dated fossil corals, radiocarbon-dated tree chronologies).

731

The radiocarbon community has a long history of standardizing the reporting of their 732 733 measurements. In 1977, Stuiver and Polach highlighted recommendations that have remained mostly unchanged (Stuiver and Polach, 1977). For chronological studies using the Libby half-life 734 (Libby et al., 1949), Stuiver and Polach recommend reporting the δ^{13} C ratio, the conventional 735 radiocarbon age (relative to CE 1950), associated error (expressed as \pm one standard deviation), 736 the estimated reservoir correction, and (optionally) the per mil depletion or enrichment with 737 respect to 0.95 NBS Oxalic acid standard (Olson, 1970). For geochemical samples, 738 dendrochronological samples, reservoir equilibria, and diffusion models, they recommend 739 reporting the δ^{13} C ratio, percent modern, and δ^{14} C and Δ^{14} C based on the Cambridge half-life of 740 5730 years (Godwin, 1962). These guidelines were further extended to include post-bomb ¹⁴C 741 data (Reimer et al., 2004) and the reporting of calibrated dates (Millard, 2014) and formed the 742 basis of the properties that were put to a vote. Given the long history of standardization, it is not 743 744 surprising that legacy radiocarbon datasets are also held at a stringent reporting level.

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For U-Th dating, the WG recommended the use of the standard proposed by Dutton et al. (2017),

with most properties recognized as essential when reporting U-series dates.

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Survey respondents also defined what information should be included when reporting the use of age modeling software. The method's name is deemed *essential* for both legacy and new datasets with most of the other properties identified as recommended. In addition, there is interest in storing ensembles of posterior draws from Bayesian approaches to ensure that the study is fully reproducible. The LiPD structure is already setup to handle multiple model output instances, allowing updates of chronologies for legacy datasets when raw data are available. They thus provide a natural container to store this information.

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Finally, respondents were asked to define some nomenclature, including the use of "present" in paleoclimate studies. Over 80% of respondents voted on keeping the concepts of age and year separated. Age is represented on a time axis starting from the "present" and counting positively back in time. On the other hand, "year" follows the Gregorian calendar and is particularly useful for studies concentrating on the past 2,000 years. Over 60% of respondents also voted on reporting years relative to CE (Common Era) rather than AD.

763

Asking for a definition of "present" yielded diverse results. Sixty-eight percent of respondents voted in favor of using 1950 as the present, following the radiocarbon convention, 7% voted in favor as defining present as the last year in a record (with no mention of uncertainty), 12% voted in favor of using 2000 as the present, while the last 13% answered "other " This last category includes the use of 1950 for radiocarbon and either something else for the other chronologies or readjusting to 1950 to stay in tune with radiocarbon and the use of either 1950 or 2000 as long as it is clearly defined with the data. In summary, there is a consensus that "present" should be defined as an absolute date (and reported in the metadata), but it should be archive-dependent,
with practitioners of U-series dating leaning towards CE 2000 and practitioners of radiocarbon
dating leaning towards CE 1950.

774

One issue in reporting ages is, again, the lack of standards. The most common standard for time 775 776 and date reporting (e.g., ISO 8601) does not accommodate for geologic time. The more recent OWL time ontology draws on the work of Cox and Richard (2015) and includes these concepts. 777 However, these authors offer no finer division of geologic time than eras. This means that the 778 779 vast majority of archived paleoclimate datasets (particularly, the totality of datasets archived on the LinkedEarth platform) would represent a single time point (the Quaternary era). To remedy 780 this gap between ISO 8601 and the OWL time representation, we hereby propose a precise 781 mechanism to report the time axis in paleoclimate datasets: 782

783

784 Time (age) = **significand** . 10^{exponent} years **direction datum**

785

Where "**significand**" and "**exponent**" are components of standard floating-point representation; "**direction**" indicates whether time flows forward (since a datum, as in the case of AD dates), or backwards (before a particular datum, as in the case of ages). "**Datum**" here refers to the origin point of the time (age) axis, which is arbitrary and (as recounted by Wolff, 2007) highly inconsistent among researchers.

791

Table 1 shows how this representation would work in practice. Note that variability in the datum for rows 1 (21 ky BP, a common date for the Last Glacial Maximum) and 4 (127 ky BP, a common date for Marine Isotope Stage 5e) could arise because of the date being reported from a radiocarbon vs. U-series chronology, and is usually impossible to infer without clarification from the original publication, or from its authors. The current proposal removes such ambiguities and can accommodate both observed and simulated datasets, potentially easing the task of modeldata comparison if both communities start adopting it.

799

800 **5.** An example: MD98-2181

This section puts these recommendations into practice on a real-world dataset: the MD98-2181 marine sedimentary record from Khider et al. (2014). The purpose is twofold: (1) illustrate how to implement these recommendations in practice and (2) draw attention to practical difficulties that may impede large-scale adoption of PaCTS v1.0.

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MD98-2181 is the most metadata-rich dataset currently available on the LinkedEarth platform since it was used as an example to further develop the LiPD framework and later the LinkedEarth Ontology. The dataset consists of measurements of Mg/Ca and δ^{18} O made on the planktic foraminifera *Globigerinoides ruber* (white, *sensu stricto* and *lato*) and δ^{18} O made on the benthic foraminifera *Cibicidoides mundulus* to infer surface and deep ocean variability in the western tropical Pacific over the Holocene. The age model is based on radiocarbon measurements for the Holocene and deglacial portion of the core.

813

Using the standards proposed for cross-archive metadata, Mg/Ca and δ^{18} O on foraminifera, radiocarbon-based chronology, and uncertainties, we calculated how many metadata properties in the essential and recommended categories were present in the MD98-2181 datasets (Figure 817 16). Since, by default, all metadata are desired, we ignored this category for the purpose of this example. In terms of its cross-archive metadata, the MD98-2181 record is nearly complete, with 818 95% of the essential metadata and 78% of the recommended metadata present in the record 819 (Figure 16). The only missing component of essential metadata is the sample thickness. For the 820 recommended category, the International Geo Sample Number (IGSN) for the sample and date at 821 which the measurements were performed (i.e., analysis date) are missing. The core IGSN should 822 be assigned by the core repository directly (e.g., Bremen Core Repository, Oregon State 823 University core repository). Both analysis dates and sample thickness are metadata readily 824 825 available at the time of collection. Although both were collected in either a physical notebook or by the instrument during analysis, they were not archived with the dataset on LinkedEarth since 826 the information was not deemed by the metadata authors as essential for reproducibility. 827

828

The paleodata for the record consists of Mg/Ca and δ^{18} O measurements on foraminifera tests 829 from sediment core subsamples. For the essential reporting of δ^{18} O on foraminifera, the MD98-830 2181 record lacks metadata regarding the taxonomy scheme being followed and equilibrium 831 offsets. In the recommended category, only the volume of sediment analyzed is missing. For 832 Mg/Ca reporting, the contamination indicator values (Mn/Ca and Fe/Ca; Khider et al., 2014) are 833 missing from the archived record in addition to the taxonomy scheme being followed. Neither 834 were deemed useful for reproducibility by the authors of the study at the time of reporting. In 835 836 the recommended category, the volume of sediment analyzed and habitat depth have not been reported. In both cases, the values are unknown, either because they were not measured during 837 sample preparation (sediment analyzed) or could not be accurately determined (habitat depth) 838 839 from previous studies in the region.

840

The MD98-2181 chronology was based on radiocarbon measurements. Ninety percent of the raw 841 radiocarbon dates used in Khider et al. (2014) were reported in Stott et al. (2004) and Stott et al. 842 (2007). The raw data necessary for the repeatability and replicability of the age model in Khider 843 et al. (2014) were re-reported in the later study. However, the archived record is missing 844 845 information about the modern fraction (F14C), the sample ID, and the matrix, which are deemed essential. The archived record is also missing most of the recommended properties, only 846 reporting the reservoir age correction (ΔR), the ensemble statistics, and the ensemble age 847 models. The last two properties are essential in the context of the Khider et al. (2014) study to 848 reproduce the age-uncertain spectral analysis. The Stott et al. (2004) and Stott et al. (2007) 849 studies are also missing the essential and recommended properties with respect to reporting of 850 raw measurements. 851

852

For uncertainty quantification, the record metadata lack the number of repeated measurements and the model parameters in the essential category, though it should be noted that the values of repeated measurements are reported in the measurement table itself. The record is complete in the recommended category.

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This example highlights the difficulty of reporting all essential metadata, especially after the study has been completed. We therefore present version 1.0 of PaCTS as an aspirational standard, one that would theoretically ensure optimal reuse of paleoclimate datasets but is difficult to observe in practice. Clearly, being aware of these requirements at the start of a study would help scientists keep track of the necessary metadata and ensure that they are reported when the dataset is digitally published (e.g., on WDS-Paleo or PANGAEA). We therefore recommend that investigators plan ahead of time which properties they intend to report, and structure their lab notebooks so this information is easier to track at the time of publication.

866 **6. Discussion**

This paper describes the first effort by the global paleoclimate community to define standards for 867 digitally archiving paleoclimate datasets. Such standards aim to make publicly archived 868 paleoclimate data more re-usable by clearly describing them with comprehensive metadata. In 869 combination with the LinkedEarth Ontology, these standards also help meet the interoperability 870 principle by using a formal, accessible, shared, and broadly applicable language for knowledge 871 representation. If the datasets are properly described using micro-data (e.g., Schema.org), they 872 873 are also findable. Together, these standards bring such datasets closer to compliance with "FAIR" principles. 874

875

876 The standards arose through collective discussions, both in-person and online, and via an innovative social platform (Gil et al 2017). The results of this collective decision-making reveal 877 an evident desire for archiving a rich set of metadata properties, with respondents identifying 878 roughly two thirds of properties (208 out of 302) as essential for new datasets. Respondents also 879 880 recognized that legacy datasets may not be as complete, so they identified less stringent requirements in order not to overlook valuable datasets. Nonetheless, respondents identified 131 881 properties as *essential* for legacy datasets, highlighting the fact that a dataset loses its usefulness 882 if too many requirements are not met. Several respondents also indicated that, while some 883 properties should theoretically be essential (or recommended), they may be hard to obtain in 884 practice and/or variable in time. These include seasonality and habitat depth of foraminifera and 885

many of the properties from TRiDaS. Furthermore, although rich metadata are always valuable,
these requirements should be balanced with the researcher's time. Scans of historical documents
or uploads of x-radiographs of archive samples would be highly valuable to the community, but
these activities are time-consuming and this use of time is rarely, if ever, incentivized by funding
agencies.

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PaCTS v1.0 is also missing several proxy systems, including loess and continental records, faunal and floral counts in lake sediments and does not incorporate recent standards such as the one developed by Courtney Mustaphi et al. (2019) for ²¹⁰Pb dating. Finally, although crosspollination was encouraged, common properties were not adequately identified across WGs, resulting in duplicates. This is especially apparent in the lake and marine sediment WGs.

897

Another salient outcome is that this first version of PaCTS can only be described as aspirational. 898 Indeed, section 5 illustrates that even in the best of circumstances (the author describing their 899 own dataset, generated less than a decade ago), the compliance rate was far from perfect. This 900 points to the need for more realistic guidelines. It is indeed apparent that many participants 901 misinterpreted what was meant by "essential." Further, the participation rate is still far below 902 what is needed for this standard to be representative of the worldwide paleoclimate community, 903 which would gain much from harmonization. How can this standard be collectively refined and 904 905 more broadly adopted? How should the standard, and its future versions, be implemented in practice? 906

907

6.1 Broadening participation

⁹⁰⁸ The genesis of PacTS v1.0 serves as a useful template for future efforts. As detailed in section 2,

the spark for the discussion came from the 2016 workshop on Paleo Data Standards. Nothing 909 replaces the immediacy of in-person communication for this sort of work. However, it would be 910 costly, carbon-intensive and unrealistic to expect large segments of the paleoclimate community 911 to travel for such an event, should it happen again. We therefore advocate that further discussion 912 take place within, or around, existing meetings. Examples include the annual meetings of the 913 American Geophysical Union and the European Geosciences Union, the Goldschmidt 914 conference, Ocean Sciences meeting, the PAGES Open Science Meeting, the International 915 Conference on Paleoceanography, meetings of the International Union for Quaternary Research, 916 917 as well as more focused meetings like WorldDendro, Karst Record, or the ASLO Aquatic Sciences Meeting. We have also found PAGES-sponsored workshops to be excellent 918 opportunities to discuss data stewardship considerations, of which reporting standards are an 919 important aspect. At the very least, an annual session at an international meeting would be useful 920 for the community to touch base and take stock of progress and challenges, but more frequent 921 interactions will be desirable until adoption reaches a critical threshold (e.g., 80% of submissions 922 to public repositories like WDS-Paleo or PANGAEA). 923

924

Assuming such meetings will take place over the next few years in many corners of the community, there is still a need for more sustained forms of communication. The virtual working groups on the LinkedEarth platform is where many of our discussions took place, and they remain available to complement to in-person discussions. Membership is open, and we encourage interested readers to join LinkedEarth so they can participate in these forums or create their own forums on a platform of their choice (traceability and transparency being of paramount importance).

932	6.2 Roadmap to standardization
933	In practical terms, we recommend that the next iteration of PaCTS use the following steps:
934	(1) The procedure for ratification is developed in tandem with major stakeholders (scientific
935	societies, data repositories, chief editors).
936	
937	(2) The proposed procedure is widely distributed to the community (e.g., through the PAGES
938	magazine, AGU and EGU communication channels, social media).
939	
940	(3) The timeline for discussion and voting is clearly indicated, and voting occurs on the
941	LinkedEarth platform.
942	
943	(4) The vote outcome is presented at a major international meeting and any additional discussion
944	is considered before the vote is certified at the meeting.
945	
946	(5) The standard is widely disseminated and encouraged by appropriate incentives (see below).
947	6.3 Implementing Emerging Standards
948	We envision two main ways to encourage the adoption of the standard. The first is to use
949	technical innovation to lower the barrier to metadata archiving; the second is to change the
950	incentive structure to make it worthwhile for researchers to adopt the standard, despite the
951	inevitable opportunity cost that comes with providing more complete data records.
952	
953	On the first point, the LinkedEarth project has recently implemented a web interface to convert
954	paleoclimate datasets into the LiPD format: the lipd.net "playground"

(http://lipd.net/playground). To promote standardization, the reporting recommendations 955 described herein will be flagged as users create LiPD files interactively on the lipd.net website, 956 pulling data and metadata from native archival formats (e.g., Excel spreadsheets). Ideally, all 957 records, especially those accepted on the LinkedEarth platform, will show their compliance rate 958 with PaCTS. This rate can be computed during creation of the LiPD file, allowing "unavailable" 959 960 as an answer for the essential fields. At present, the lipd.net playground displays the rate of required fields that have been entered, but is not set up to track archive or proxy-specific 961 completeness, although this is possible with further development. The "unavailable" category 962 serves two purposes: (1) to encourage researchers to gather these metadata during their next 963 study and (2) to investigate how many of these essential properties are reported in practice. 964 Alternatively, LinkedEarth could appoint a Board of Data Editors to approve the datasets for 965 upload onto the platform. The Board presents several advantages over an automatic process: (1) 966 to answer specific questions, therefore taking into consideration the intricacies of a dataset; (2) to 967 identify needed changes to the reporting standards faster; and (3) to assist the community with 968 the online web service when needed. The major drawback is the volunteer time of the Board of 969 Data Editors. In our experience, the time of researchers is already stretched thin, and they have 970 971 little incentive to commit more of it to the relatively thankless task of standardization.

972

How might the reward structure be changed? There are essentially two levers to activate. The first is funding agencies. In the United States, for instance, the National Science Foundation funds the vast majority of paleoclimate research. While the agency now requires a data management plan to be submitted for each proposal, its reporting guidelines are very broad. They could be made more specific, and point paleoclimate researchers to the latest version of PaCTS. The European Research Council similarly supports Open Science, but with far less specific guidelines than PaCTS v1.0. To the best of our knowledge, the situation is similar for other countries (e.g., Canada, Australia). We therefore call on funding agencies to either endorse this standard or propose a meaningful alternative.

982

983 The second lever is publishers and editors: while each publishing house encourages digital data archiving to varying degrees, the decision of what (meta)data to include is ultimately up to the 984 author, and often fails to consider the long-term value proposition of the dataset. Publishers 985 could help ensure that the present standard is, at the very least, encouraged, if not mandatory. In 986 particular, the American Geophysical Union and Copernicus publishers recently endorsed 987 requirements to make data FAIR. Affiliated journals could use their leverage to promote more 988 stringent reporting standards. As an example, the recent PAGES 2k special issue of the journal 989 Climate of the Past piloted the implementation of open-data practices, which included some 990 reporting standards, and reported the challenges faced when requiring such practices (Kaufman 991 et al., 2018). Another avenue for promoting best practices, including adoption of reporting 992 standards, is through professional paleoscience organizations such as PAGES and INQUA. 993

994

We expect the present reporting standard to evolve to meet the needs of the paleoclimate community. It is our hope that this publication will stimulate volunteers to join the effort and organize discussions at all community levels; there can be no community standard without community involvement. We are confident that improving paleoclimate data standards will promote collaboration on international data syntheses and encourage the development of software based on the new standards. In turn, such software will reduce the time to science, by 1001 compressing the time researchers spend on the menial task of data wrangling.

1002 Acknowledgments, Samples, and Data

- 1003 Code and data to reproduce the figures of this article are available on GitHub and released on
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 <u>overview/</u>
- **Figure 1**. Timeline of the community elicitation for best practices in paleoclimate data reporting.
- 1166 The Workshop on Paleoclimate Data Standard marks the official beginning of the endeavor.

- 1167 PaCTS collects responses from the LinkedEarth platform, Twitter polls, and survey up to
- 1168 November 2017.
- **Figure 2**. Example of polls on a. the LinkedEarth platform and b. Twitter (@Linked_Earth)
- 1170 **Figure 3.** Example of a survey question for a new dataset. The histogram represents the number
- 1171 of votes on each platform (orange: LinkedEarth, purple: Twitter, and green: Google survey). The
- pie chart represents the fraction of the votes for essential (green), recommended (pink), and
- 1173 desired (blue).
- 1174 **Figure 4.** Same as Figure 3 for a legacy dataset.
- **Figure 5.** Mind map of the various properties identified by the WGs and associated vote. Colors
- 1176 represent the different WGs. Parentheses indicate a different reporting standard for legacy 1177 datasets when different from new datasets. Available online at:
- 1178 https://coggle.it/diagram/WqMd49MJtB8DbqfH/t/community-standards-for-paleoclimate-data-
- 1179 and-metadata.
- 1180 Figure 6. Mosaic plots for a. new datasets and b. legacy datasets showing the number of
- essential, recommended, and desired metadata for the various WGs. The height of the bar
- represents the fraction of total occurrences for essential (e), recommended (r), and desired (d)
- 1183 votes, while the width of the bar represents the number of properties voted on in each WG.
- **Figure 7.** Mind map of the various properties identified by the cross-archive WG and associated
- vote. Color is the same as in Figure 5. Parentheses indicate recommendations for legacy datasets
- 1186 when different from new datasets. Available online at:
- 1187 https://coggle.it/diagram/W4W9podcxp86PPvf/t/cross-archive-metadata
- 1188 **Figure 8.** Mind map of the various properties identified by the ice core archives WG and
- associated vote. Color is the same as in Figure 5. Parentheses indicate recommendations for
- 1190 legacy datasets when different from new datasets. Available online at:
- 1191 https://coggle.it/diagram/W4XNNeGhIngfjHzB/t/historical-documents
- 1192 **Figure 9.** Mind map of the various properties identified by the lake sediments archives WG and
- associated vote. Color is the same as in Figure 5. Parentheses indicate recommendations for
- 1194 legacy datasets when different from new datasets. Available online at:
- 1195 https://coggle.it/diagram/W4h9m-GhIjjbm3yX/t/lake-sediments
- 1196 **Figure 10.** Mind map of the various properties identified by the marine sediments archives WG
- and associated vote. Color is the same as in Figure 5. Parentheses indicate recommendations for
- 1198 legacy datasets when different from new datasets. Available online at:
- 1199 https://coggle.it/diagram/W4iIkodcxlDKTK6v/t/marine-sediments
- 1200 **Figure 11.** Mind map of the various properties identified by the speleothem archives WG and
- associated vote. Color is the same as in Figure 5. Parentheses indicate recommendations for
- 1202 legacy datasets when different from new datasets. Available online at:
- 1203 https://coggle.it/diagram/W4gwj-GhIl4VmfYP/t/speleothem

- 1204 **Figure 12.** Mind map of the various properties identified by tree-based archives WG and
- associated vote. Color is the same as in Figure 5. Parentheses indicate recommendations for
- 1206 legacy datasets when different from new datasets. Available online at:
- 1207 https://coggle.it/diagram/W4huaYdcxhdzTB9z/t/trees
- 1208 **Figure 13.** Mind map of the various properties identified by the documentary archives WG and
- associated vote. Color is the same as in Figure 5. Parentheses indicate recommendations for
- 1210 legacy datasets when different from new datasets. Available online at:
- 1211 https://coggle.it/diagram/W4XNNeGhIngfjHzB/t/historical-documents
- 1212 **Figure 14.** Mind map of the various properties identified by the uncertainties WG and associated
- vote. Color is the same as in Figure 5. Parentheses indicate recommendations for legacy datasets
- 1214 when different from new datasets. Available online at:
- 1215 https://coggle.it/diagram/W4gttodcxjfvSst0/t/uncertainties
- 1216 **Figure 15.** Mind map of the various properties identified by the chronologies WG and associated
- vote. Color is the same as in Figure 5. Parentheses indicate recommendations for legacy datasets
- 1218 when different from new datasets. Available online at:
- 1219 https://coggle.it/diagram/W4hzXeGhIi5Fm0q7/t/chronologies
- 1220 Figure 16. Radar plot showing the completeness of the metadata reporting for core MD98-2181
- 1221 (Khider et al., 2014) for properties considered a. essential and b. recommended in the current
- study. The axis refers to the working group standards recommendation applicable to the record.

Reported	Significand	Exponent	Direction	Datum
Age/year in				
manuscript				
21 ka BP	21	3	before	1950 CE
1816 AD	1816	0	since	0 CE ¹
2.7 Ma	2.7	6	before	1950 CE
127 ka BP	127	3	before	2000 CE

1224 **Table 1.** Illustration of our proposed time representation with four time points. The first column

1225 gives examples of reported age/year in a paleoclimate paper while the last four columns show an

1226 implementation of the representation proposed here.

Figure 1.

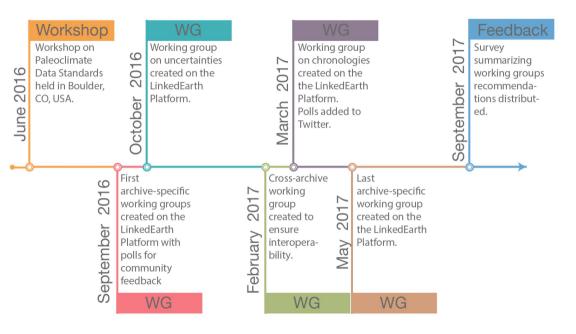


Figure 2.

For stable isotopes in foraminifera, should size fraction be:

You voted for "Recommended Metadata" on 7 March 2017 at 15:50. You can change your vote by clicking a different answer below.

Essential Metadata

Recommended Metadata

Desired Metadata

I want to revoke my vote

There were 4 votes since the poll was created on 15:48, 7 March 2017.



b.

2

2

0

Figure 3.

For new datasets, should the depth/distance/position in the archive be considered essential, recommended, or desired?

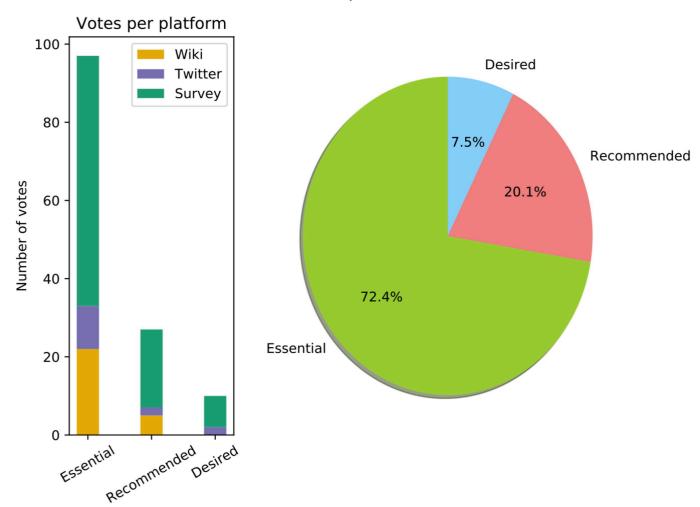


Figure 4.

For legacy datasets, should the depth/distance/position in the archive be considered essential, recommended, or desired?

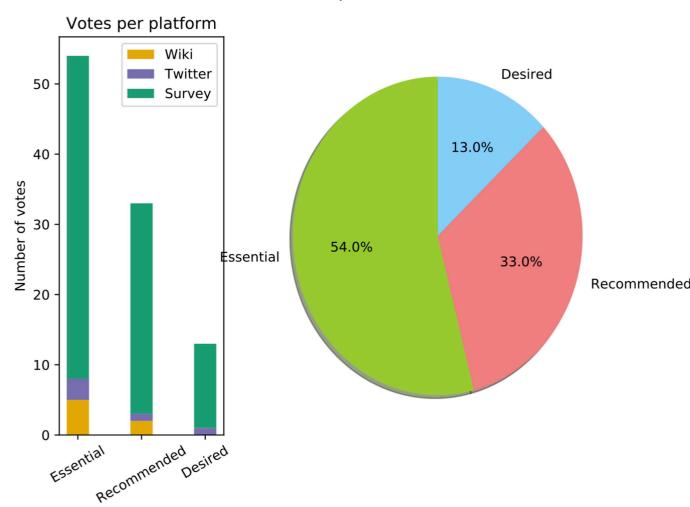
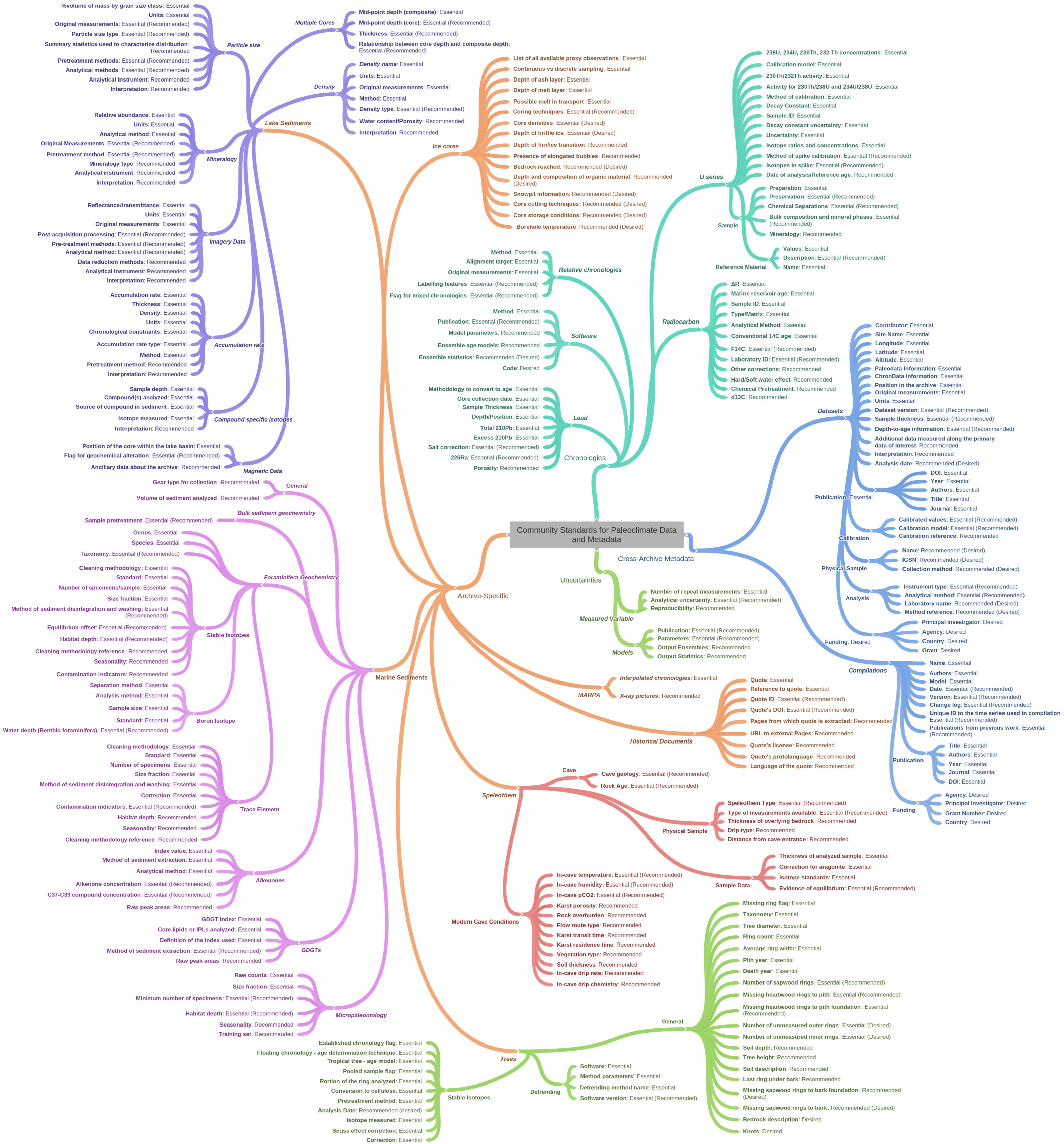


Figure 5.



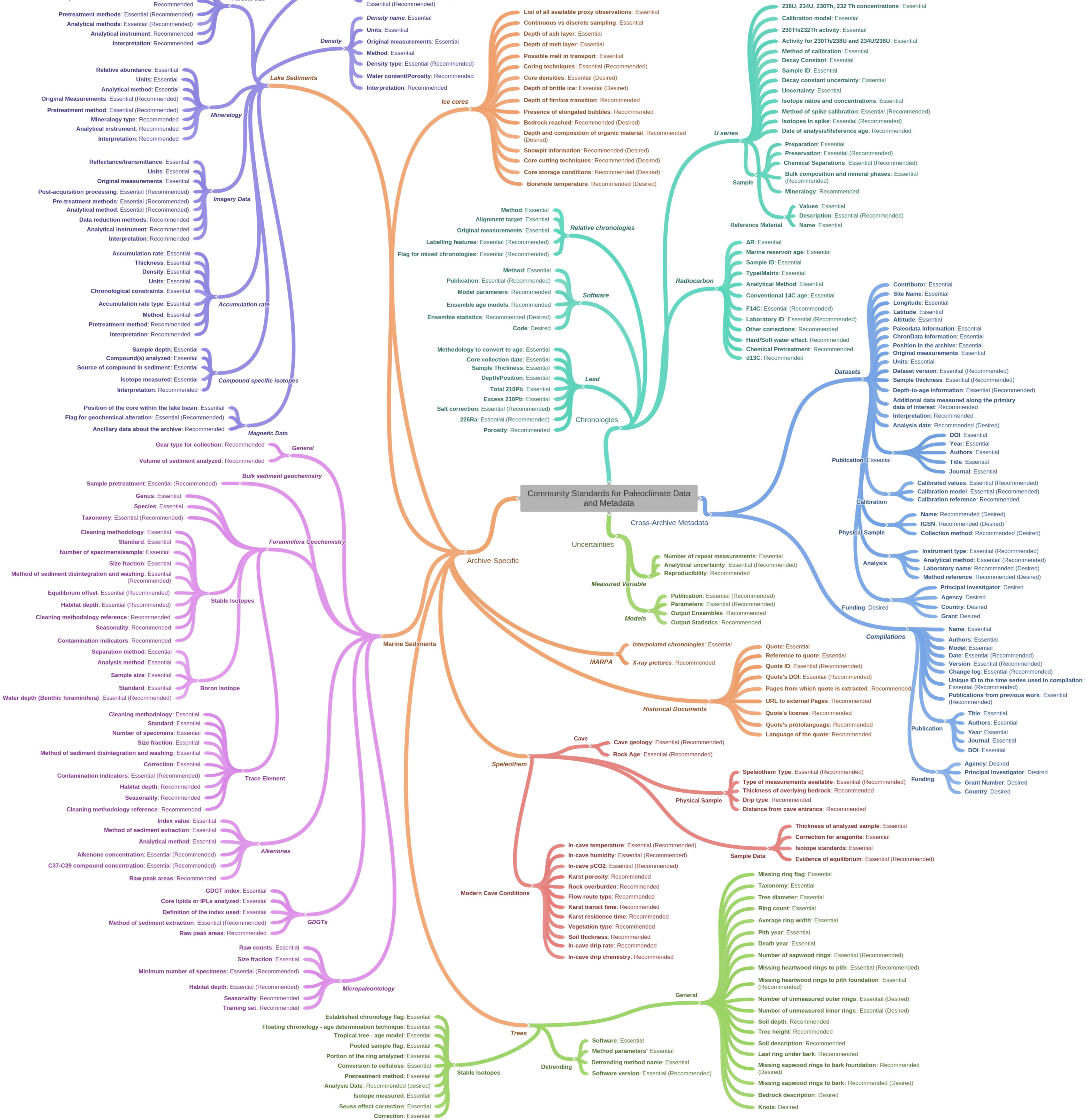
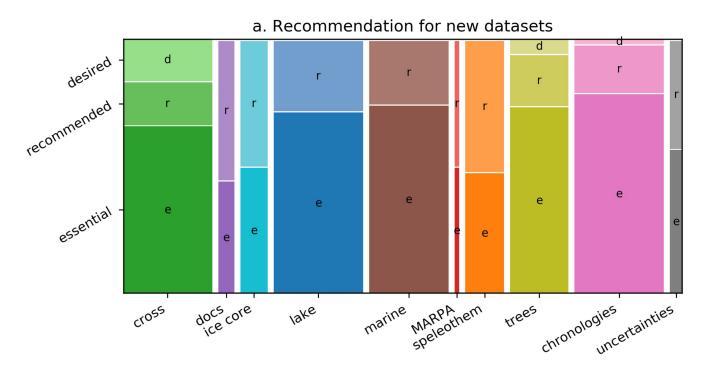


Figure 6.



b. Recommendation for legacy datasets

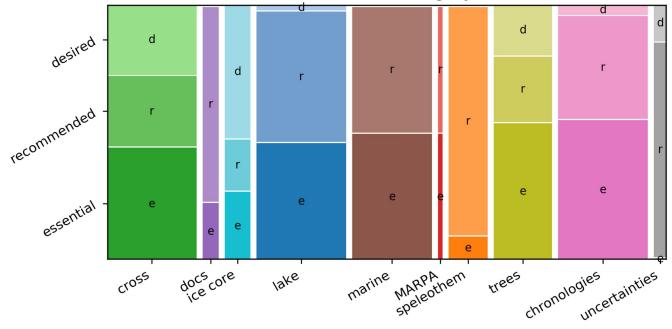


Figure 7.

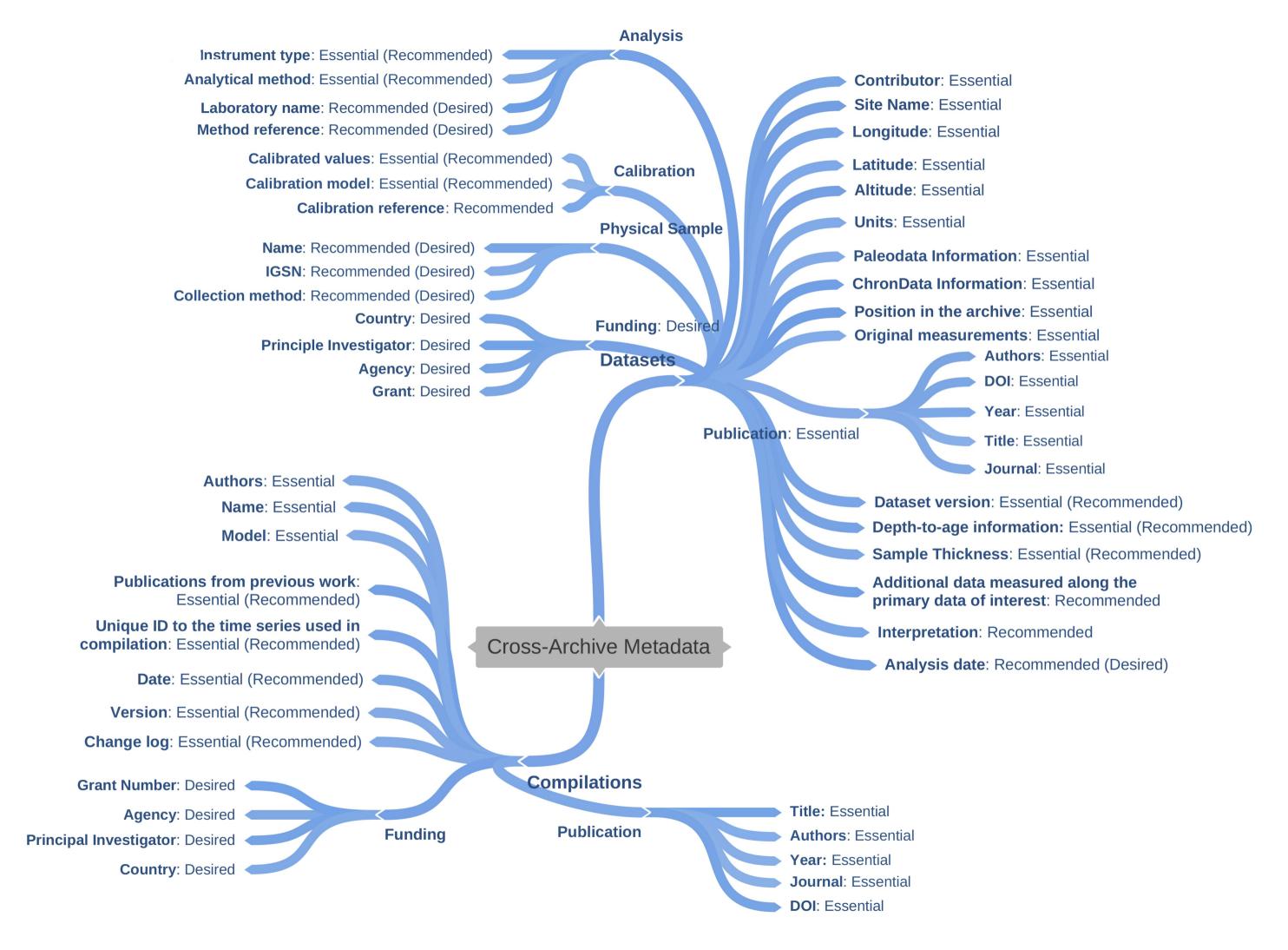
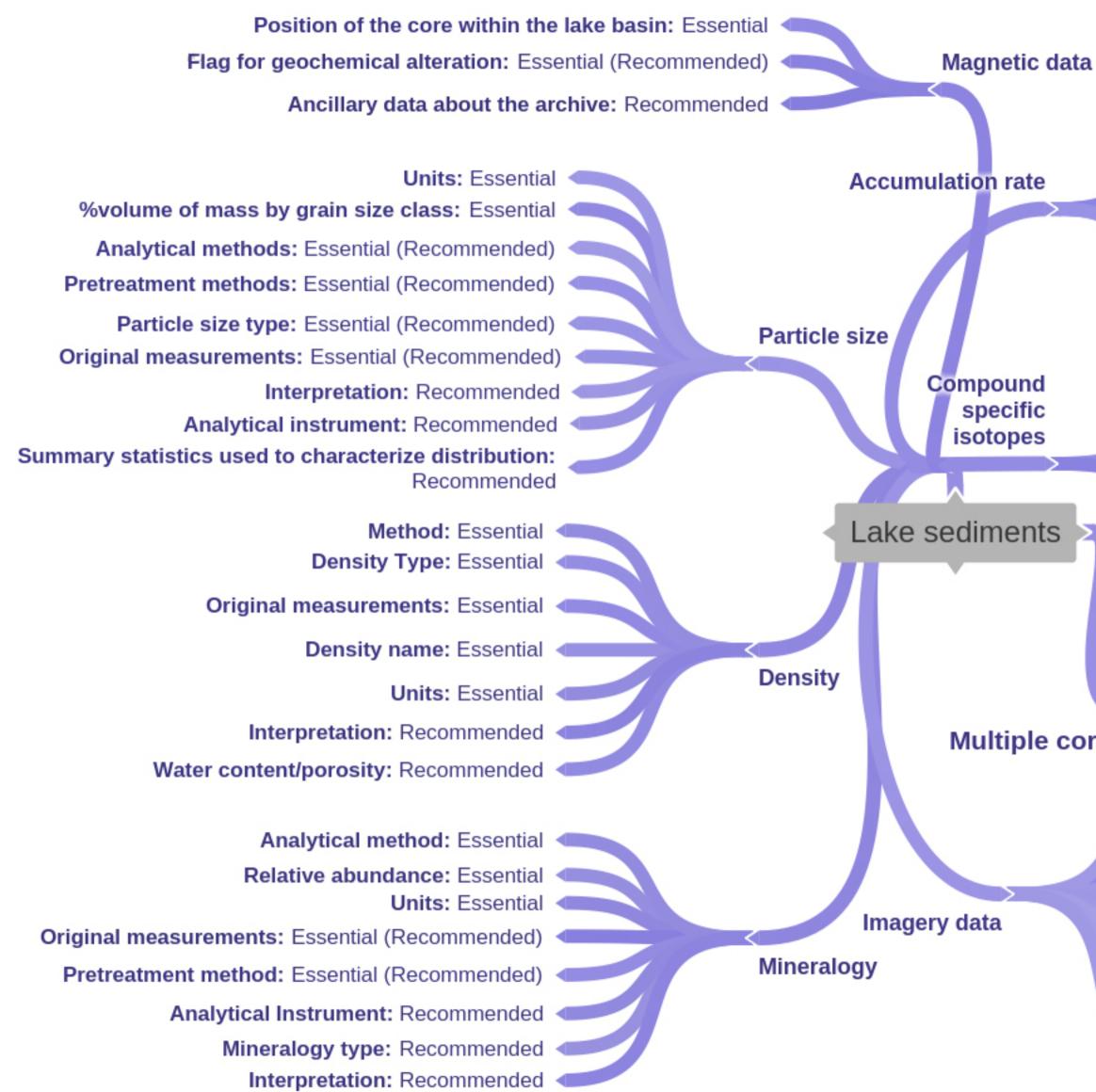


Figure 8.

Ice Cores

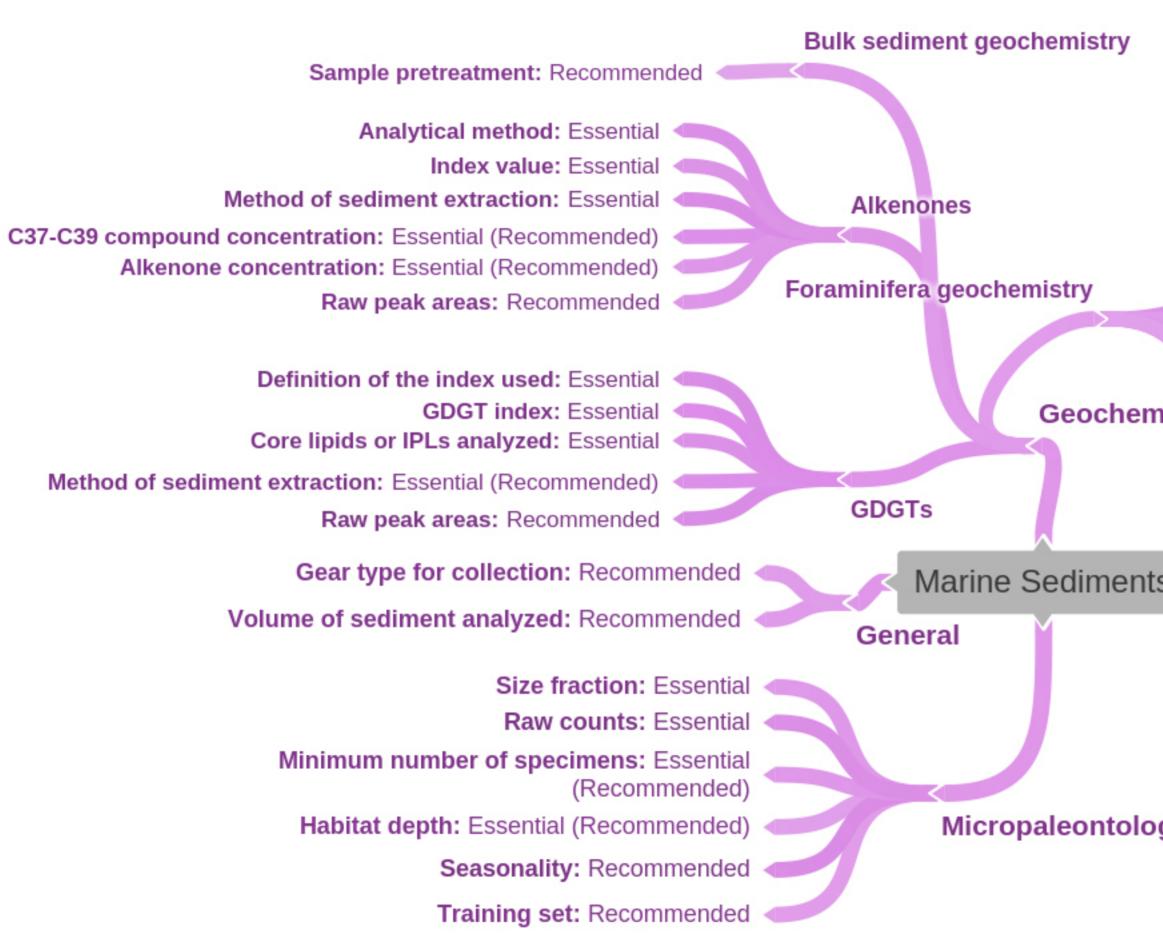
- **Continuous vs discrete sampling**: Essential
- **Depth of melt layer:** Essential
- List of all available proxy observations: Essential
- **Depth of ash layer:** Essential
- **Possible melt in transport**: Essential
- **Coring techniques**: Essential (Recommended)
- **Core densities**: Essential (Desired)
- **Depth of brittle ice:** Essential (Desired)
- **Depth of firn/ice transition**: Recommended
- **Presence of elongated bubbles:** Recommended
- **Core storage conditions**: Recommended (Desired)
- **Borehole temperature**: Recommended (Desired)
- **Snowpit information**: Recommended (Desired)
- **Bedrock reached:** Recommended (Desired)
- **Depth and composition of organic material:** Recommended (Desired)
- **Core cutting techniques**: Recommended (Desired)

Figure 9.



Method: Essential Chronological constraints: Essential **Density:** Essential Accumulation rate: Essential Thickness: Essential Units: Essential Accumulation rate type: Essential Interpretation: Recommended Pretreatment method: Recommended Isotope measured: Essential Source of compound in sediment: Essential Sample depth: Essential Compound(s) analyzed: Essential Interpretation: Recommended Mid-point depth (composite): Essential Mid-point depth (core): Essential (Recommended) Thickness: Essential (Recommended) Relationship between core depth and composite depth: Multiple cores Essential (Recommended) Original measurements: Essential Reflectance/transmittance: Essential **Units:** Essential Post-acquisition processing: Essential (Recommended) Pre-treatment methods: Essential (Recommended) Analytical method: Essential (Recommended) Data reduction methods: Recommended Analytical instrument: Recommended Interpretation: Recommended

Figure 10.



		Standard: Essential		
		Size fraction: Essential		
		Method of sediment disintegration and washing: Essential		
		Number of specimens: Essential		
		Cleaning methodology: Essential		
		Correction: Essential		
		Contamination indicators: Essential (Recommended)		
		Habitat depth: Recommended		
		Seasonality: Recommended		
		Cleaning methodology reference: Recommended		
		Standard: Essential		
		Sample size: Essential		
	Boron isotopes	Analysis method: Essential		
nistr		Separation method: Essential		
		Water depth (benthic): Essential (Recommended)		
		Number of specimens/sample: Essential		
		Standard: Essential		
		Cleaning methodology: Essential		
s		Size fraction: Essential		
		Method of sediment disintegration and washing: Essential (Recommended)		
	Stable Isotopes	Equilibrium offset: Essential (Recommended)		
gy		Habitat depth: Essential (Recommended)		
		Seasonality: Recommended		
		Cleaning methodology reference: Recommended		
	Genus: Essential			
	Species: Essential			
		tial (Recommended)		

Figure 11.

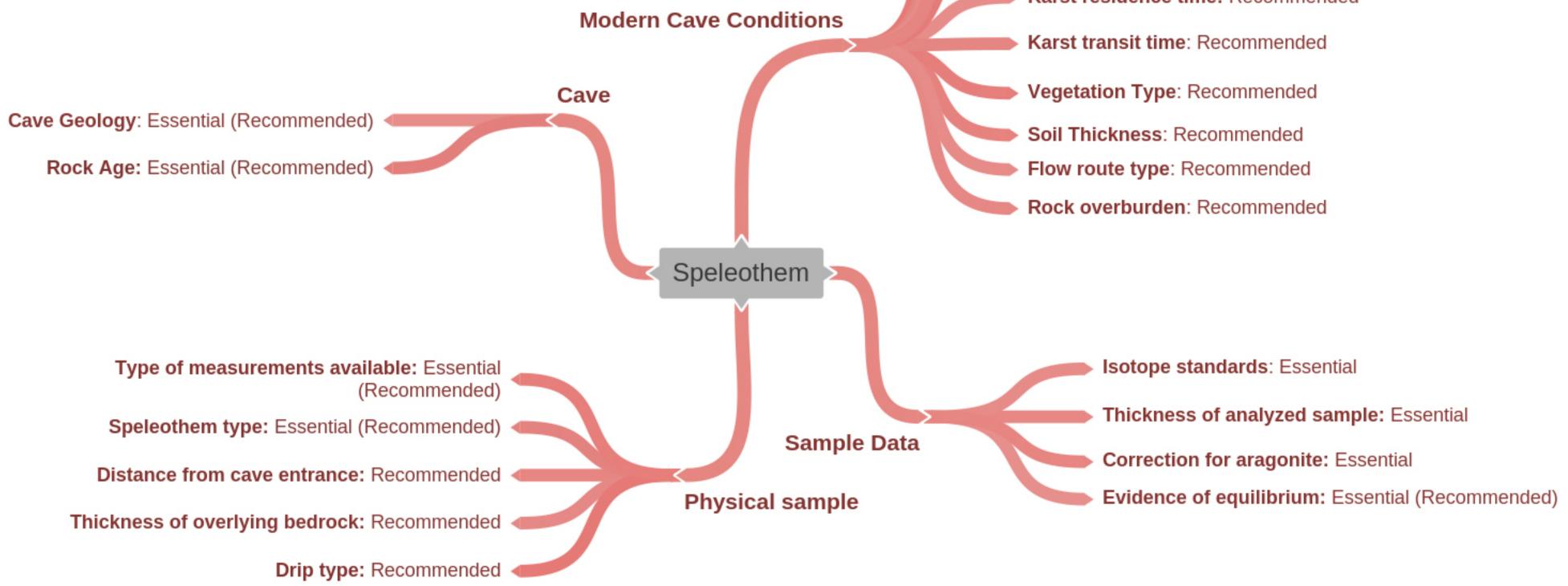




Figure 12.



Missing sapwood rings to bark: Recommended Missing sapwood rings to bark foundation:

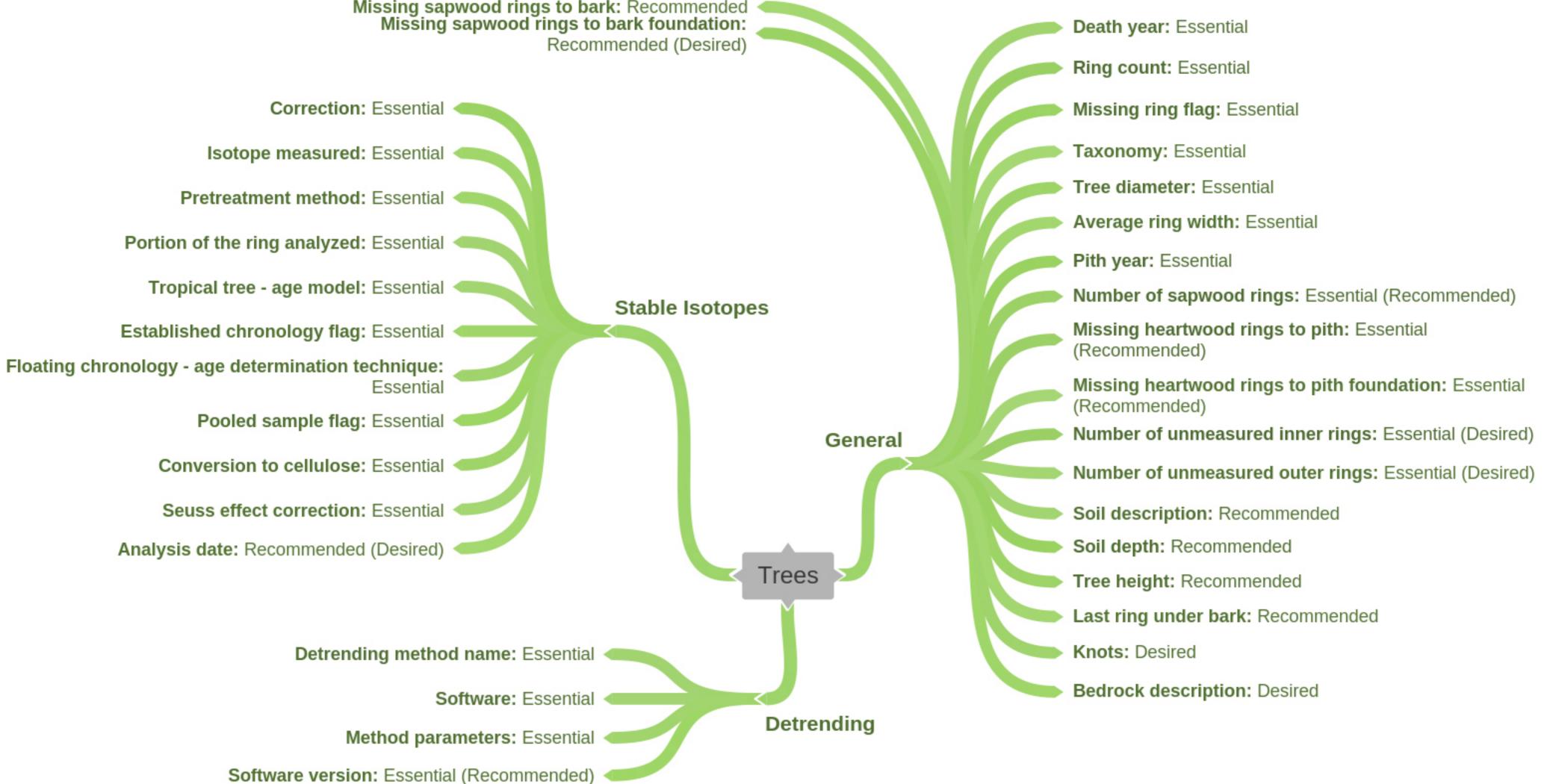
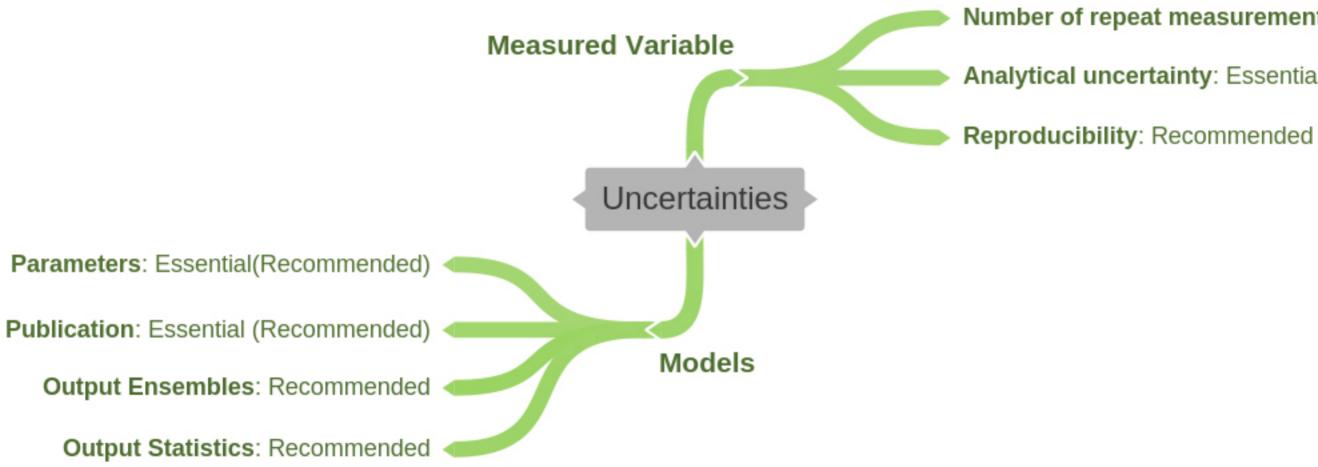


Figure 13.

Historical Documents

Reference to quote: Essential **Quote**: Essential **Quote ID**: Essential (Recommended) **Quote's DOI:** Essential (Recommended) **URL to external pages**: Recommended Language of the quote: Recommended Quote's license: Recommended Quote's protolanguage: Recommended Pages from which quote is extracted: Recommended

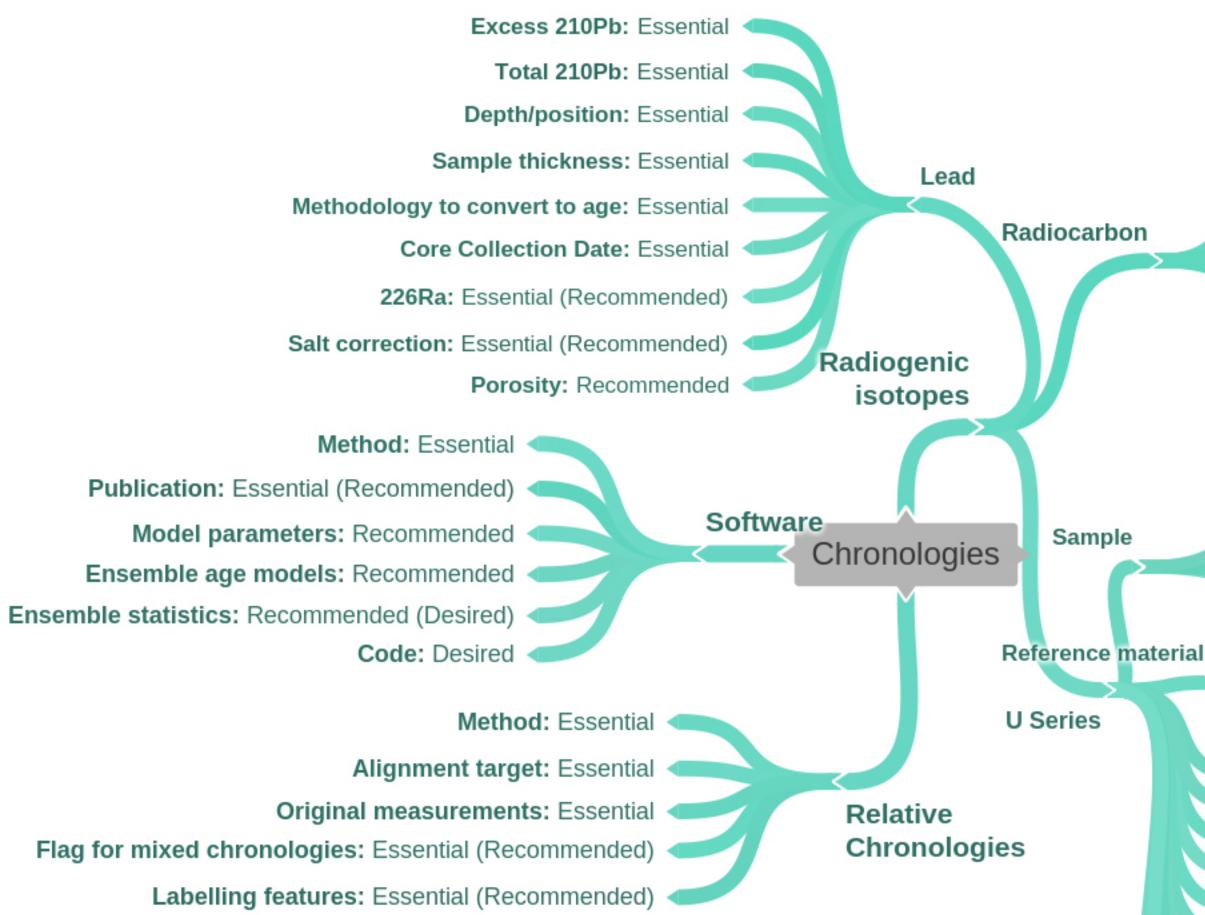
Figure 14.



Number of repeat measurements: Essential

- Analytical uncertainty: Essential (Recommended)

Figure 15.



 ΔR : Essential

Analytical method: Essential Marine reservoir age: Essential Sample ID: Essential Type/Matrix: Essential Conventional 14C age: Essential F14C: Essential (Recommended) Laboratory ID: Essential (Recommended) Other Corrections: Recommended Hard/soft water effect: Recommended Chemical pretreatment: Recommended d13C: Recommended

Preparation: Essential Preservation: Essential (Recommended) Bulk composition and mineral phases: Essential (Recommended) Chemical separations: Essential (Recommended) Mineralogy: Recommended Values: Essential Name: Essential

Description: Essential (Recommended)

238U, 234U, 230Th, 232Th concentrations: Essential Decay constant: Essential Calibration model: Essential 230Th/232Th activity: Essential Activity for 230Th/238U and 234U/238U: Essential Method of calibration: Essential Sample ID: Essential Decay constant uncertainty: Essential Uncertainty: Essential Isotope rations and concentrations: Essential Isotopes in spike: Essential (Recommended) Method of spike calibration: Essential (Recommended) Date of analysis/reference age: Recommended

Figure 16.

a. Essential

b. Recommended

