Roinn Cumarsáide, Gníomhaithe ar son na hAeráide & Comhshaoil
Department of Communications, Climate Action & Environment

Geological Survey
Suirbhéireacht Gheolaíochta
Ireland | Éireann

Research Programme
- Short Calls, Final Report -

Lead Applicant Name	Laia Comas Bru
Email	laia.comasbru@ucd.ie
Host Organisation name	University College Dublin
Project Title	Developing toolkit for model evaluation using speleothem isotope data
Contract Number	2017-sc-056

Date: 1st November 2018

This report covers the period November 1st 2017 to October 31st 2018

2. (a) Project information:

<u>Final project report (*max **2500**words, excluding figures and headings*)</u>:

- *<u>Progress</u>* of objectives and scientific/engineering targets beyond the state of the art & *<u>methods</u>* used

All the project targets and milestones expected of the project have progressed substantially and most have been achieved in full. These include the following:

(Note: Objectives outlined in the proposal are in italics below)

1-4M:

- *Finalising our list of identified records, which currently comprises 520 records (fully accomplished)*

Expansion of list of identified records from 520 to 720 records

- *Data compilation of non-publicly accessible records (only 169 records are archived in open repositories). (fully accomplished)*

The first compilation comprises 366 individual speleothem records and 10 composites from 172 cave systems worldwide (including 5 unpublished records)

- Quality control of compiled records before they are uploaded to the SISAL database. This includes liaising with data owners to ensure the completeness of the records submitted to SISAL *(fully accomplished)*

A set of automatized checks has been created over the course of this project in collaboration of the research database manager employed by our partner Sandy Harrison at the University of Reading. These scripts are updated on an on-going basis when mistakes are identified while analysing the database. These scripts have been shared with the SISAL regional coordinators now in charge of ensuring that the records are uploaded into the database mistake-free. The original investigators producing the speleothem records have been contacted whenever possible to check the quality of their data being entered into SISAL.

5-7M:

- *Continued data compilation and final upload of records to the SISAL database (fully accomplished)*

The first version of the SISAL database is already published and data compilation for SISAL_v2 is on-going. Only a fraction of the published records are in SISAL_v1 and we aim to published a more complete second version of the database by the end of 2019.

- *Preliminary analyses of the SISAL database (fully accomplished)*

Analyses of the SISAL database started in month 5 and are still on-going (See comments below).

- *Draft of dataset documentation paper (fully accomplished)*

Our first project deliverable, the dataset documentation paper, was submitted to Earth Systems Data (IF: 6.696) for publication at the end of February (month 4).

- *Draft of analysis paper (in progress)*

The analyses paper will be submitted after the end of this project. Some challenges on how to deal with the data-model comparison aspect of this study have delayed its submission. Preliminary analyses of the database which had already started in the first four months of project has continued. These have resulted in the development of specially designed scripts for statistical analysis of the database as well as its evaluation in terms of temporal and spatial coverage, resolution and variability. Some challenges regarding the temporal and spatial coverage of data as well as incorporation of uncertainty and interdependency of signals are currently being addressed. To do so, more sophisticated statistical approaches are needed, and currently new scripts are being developed for signal analysis as well as uncertainty analysis and propagation using Monte Carlo simulations. This is taking more than anticipated as a result of the objectives added during the course of this project and also because the contract of the research assistant employed in this project ended in August (2 months before completion of the project). Part of these analyses are included in an output not originally planned (the regional paper in task 5).

In addition to this, the PI of this project obtained external funding (RIA Charlemont award) to visit Prof Sandy Harrison (co-PI of this project; University of Reading, UK) and Dr Martin Werner (AWI, Germany) to benefit from Sandy's expertise in analysing databases and Martin's research with palaeoclimate modelling. This external award contributed to the task 4 listed in the products of this project. The start of this task 4 was outlined in the proposal for months 5-7. In addition to this, the PI of this project attended the 3rd SISAL workshop in Agadir (Morocco) in October 2018, where there was a hands-on session of data analyses towards this publication.

- *Dissemination of SISAL results to the wide speleothem and modelling community at the EGU General Assembly 2018 (fully accomplished)*

Our abstract to present the preliminary results of this project was accepted for the European Geosciences Union General Assembly's session "*CL1.17 - The speleothem archive: understanding processes and interpreting Quaternary climate change*" and was presented on Thursday 12th April in Vienna (Austria).

8-10M:

- *Finalisation and submission of dataset documentation paper to Earth Systems Data (fully accomplished)*

The dataset documentation paper, was submitted to Earth Systems Data (IF: 6.696) for publication at the end of February (month 4), accepted for publication 21 August and published on 14 September 2018 (month 11). The PI and the research assistant employed by this project are the 2nd and 3rd authors. See: https://www.earth-syst-sci-data.net/10/1687/2018/essd-10-1687-2018.html. The database has been made publicly available by loading it to the University of Reading repository (http://researchdata.reading.ac.uk/147/) and the widely used paleoclimate repository curated by the NOAA (https://www.ncdc.noaa.gov/paleo-search/study/24070)
Along with the database, we have supplied a set of python/R codes to create the relational database from flat csv files. This will increase the usability of the database by researchers that are not familiar with MySQL software. These scripts are available at the University of Reading repository linked above.

- *Finalisation and submission of analysis paper to Nature Climate Change or Climate of the Past (in progress)*

See comment above on the challenges faced with the analyses for this paper. A draft of this paper is currently planned for December 2018.

In addition to the project targets, some new objectives have been included, as follows:

New objectives (fully accomplished)

- Apart from the planned dissemination of SISAL results at the EGU General Assembly 2018, an abstract was submitted to and accepted for PEN (Past Earth Network) conference 2018 and our poster demonstrating preliminary results of this project was presented on June 19th in University of Leeds, Leeds, UK.
- The research assistant attended GeoEnv 2018 conference and short course in Belfast, Northern Ireland, UK, 2-6 July 2018, to complement the computational statistical skills required for the tasks related to the analyses of the database.

New objectives (in progress)

- The SISAL working group members decided to publish additional regional papers in the "Speleothem Records and Climate" Special Issue of the journal Quaternary. Both, the PI and the research assistant are co-authors of the paper presenting the data for Western Europe: "*The Potential of Speleothems from Western Europe as Recorders of Regional Climate: a Critical Assessment of the SISAL Database* (Lechleitner et al.)". This paper is now in review and its pre-print is available at: https://www.preprints.org/manuscript/201809.0246/v1
- In addition to the data analysis mentioned in the project proposal, the SISAL working group decided to develop standardised chronologies using different age-model methodologies for the records in the database (SISAL_chronology). PI and research assistant are involved in implementation of OxCal age modelling methodology. This age-depth model uses Bayesian formulation and Markov Chain Monte Carlo implementation to construct accurate age models and has not been widely used in speleothem age models so far. The results of OxCal and other age models will be published in an additional paper that will compare the pros and cons of these different approached applied to speleothem-based palaeoclimate series. The research assistant employed in this project spent a considerable amount of time automatizing the implementation of OxCal in batch (still in progress). Due to the time and effort needed to re-run 380+ age models with 5 different methodologies, the paper presenting these results will not be submitted until Spring 2019. Both the PI and the research assistant are involved in this paper lead by Kira Rehfeld (University of Heidelberg).

Implementation (please include any issues with timelines, milestones, management etc. or deviations from the original implementation plan)

- Despite the delay in employing the research assistant due to administrative difficulties and time constraints, all objectives were accomplished according to or ahead of the proposed timeline.
- The analyses of the database is going slower than expected. As a result of that the paper will be submitted after the end of this project.

- Outputs (please provide a short description *and* complete the table below)

Publications

- The dataset documentation paper entitled "The SISAL database: a global resource to document oxygen and carbon isotope records from speleothems" has been published at Earth System Science Data (https://doi.org/10.5194/essd-10-1687-2018)
- A paper on the Western Europe section of the database is submitted to the "Speleothem Records and Climate" Special Issue (Quaternary) and is currently under review (https://www.preprints.org/manuscript/201809.0246/v1)

Data

- The finalised dataset (SISAL database Version 1.0) has been lodged in the University of Reading Research Data Archive (http://dx.doi.org/10.17864/1947.147) as well as in the NOAA NCEI Paleodata Center (https://www.ncdc.noaa.gov/paleo-search/study/24070)

Conference contributions

- A poster entitled "Preliminary results of the SISAL database" was presented in EGU General Assembly 2018, Vienna, Austria, April 12th, 2018.
- A poster entitled "Preliminary results of the SISAL database" was presented in PEN 2018 (Past Earth Network) Conference, University of Leeds, Leeds, UK, June 19th, 2018.

Task No.	Deliverable description	Planned delivery (as per proposal)	Date of delivery
1	Data synthesis product	Finished in month 7,	Data synthesis product finished in month 4 and published/released in month 11.
2	EGU presentation of preliminary results	Month 6	Accomplished in month 6
3	Publication of database paper	Month 10	Accomplished in month 11
4	Publication of analysis paper	Month 10	To be submitted after the end of this project (month 13-14)
5	Publication of a paper on the Western Europe section of the database in the "Speleothem Records and Climate" Special Issue (Quaternary)	(not in the proposal)	Manuscript submitted and accepted for review in month 11.
6	Presentation of preliminary results in PEN 2018	(not in the proposal)	Accomplished in month 8
7	Publication of a paper on age models (SISAL chronologies)	(not in the proposal)	After the end of project (estimated submission Spring 2019)

Publications to date: *Please use format below and provide a copy of the presentation*

[Journal Paper] Atsawawanunt, K.; **Comas-Bru, L.; Amirnezhad Mozhdehi, S.;** Deininger, M.; Harrison, S. P.; Baker, A.; Boyd, M.; Kaushal, N.; Ahmed, S. M.; Arienzo, M.; Brahim, Y. A.; Bajo, P.; Braun, K.; Burstyn, Y.; Chawchai, S.; Duan, W.; Hatvani, I. G.; Hu, J.; Kern, Z.; Labuhn, I.; Lachniet, M.; Lechleiter, F. A.; Lorrey, A.; Pérez-Mejías, C.; Pickering, R.; Scroxton, N.; and SISAL Working Group Members (2018) "The SISAL database: a global resource to document oxygen and carbon isotope records from speleothems" *Earth System Science Data*

[Journal Paper] Lechleitner, F.; **Amirnezhad-Mozhdehi, S.;** Columbu, A.; **Comas-Bru, L.;** Labuhn, I.; Pérez-Mejías, C.; Rehfeld, K. (2018) "The Potential of Speleothems from Western Europe as Recorders of Regional Climate: a Critical Assessment of the SISAL Database" (under review). Preprints 2018, 2018090246 (doi: 10.20944/preprints201809.0246.v1).

[Conference Publication] **Comas-Bru, L; Amirnejad Mozhdehi, S;** Harrison, S; and SISAL members (2018) Preliminary results of the SISAL database. EGU General Assembly 2018 – Geophysical Research Abstracts EGU2018-16650, Vienna, Austria , 12-APR-18

[Conference Publication] **Comas-Bru, L.; Amirnezhad Mozhdehi, S;** Harrison, S, Werner M.; Scroxton, N; and SISAL members (2018) Preliminary results of the SISAL database. PEN (Past Earth Network) Conference, University of Leeds, Leeds, UK.

4. Data/outputs submitted with final report *(please list the documents, presentations, datasets etc. submitted with this report)*

- **a.** PDF of the SISAL database paper (Atsawawaranunt et al., 2018)
- **b.** PDF of the preprint of the Western Europe regional paper (Lechleitner et al., in review)
- **c.** PDF of the poster presented at EGU2018 (Vienna, April 2018)
- **d.** PDF of the poster presented at PEN Conference (Leeds, June 2018)

SUPPLEMENTARY MATERIAL

(This section will be included in your published report unless otherwise instructed. If you have a published report, publication, etc. you may include it here).

Earth Syst. Sci. Data, 10, 1687–1713, 2018
https://doi.org/10.5194/essd-10-1687-2018

Open Access Earth System Science Data

The SISAL database: a global resource to document oxygen and carbon isotope records from speleothems

Kamolphat Atsawawaranunt[1], Laia Comas-Bru[2], Sahar Amirnezhad Mozhdehi[2], Michael Deininger[2,3], Sandy P. Harrison[1], Andy Baker[4], Meighan Boyd[5], Nikita Kaushal[6], Syed Masood Ahmad[7,24], Yassine Ait Brahim[8], Monica Arienzo[9], Petra Bajo[10], Kerstin Braun[11], Yuval Burstyn[12,13], Sakonvan Chawchai[14], Wuhui Duan[15], István Gábor Hatvani[16], Jun Hu[17], Zoltán Kern[16], Inga Labuhn[18], Matthew Lachniet[19], Franziska A. Lechleitner[6], Andrew Lorrey[20], Carlos Pérez-Mejías[21], Robyn Pickering[22], Nick Scroxton[23], and SISAL Working Group Members[*]

[1]Centre for Past Climate Change and School of Archaeology, Geography & Environmental Sciences, Reading University, Whiteknights, Reading, RG6 6AH, UK
[2]School of Earth Sciences, University College Dublin, Belfield, Dublin 4, Ireland
[3]Institute of Geosciences, Johannes-Gutenberg-University Mainz, Johann-Joachim-Becher-Weg 21, 55128 Mainz, Germany
[4]School of Biological, Earth and Environmental Sciences, University of New South Wales, Kensington 2052, Australia
[5]Department of Earth Sciences, Royal Holloway University of London, Egham, Surrey, TW20 0EX, UK
[6]Department of Earth Sciences, University of Oxford, South Parks Road, Oxford, OX1 3AN, UK
[7]CSIR – National Geophysical Research Institute, Uppal Road, 500 007 Hyderabad, India
[8]Institute of Global Environmental Change, Xi'an Jiaotong University, Xi'an, Shaanxi, China
[9]Division of Hydrologic Sciences, Desert Research Institute, 2215 Raggio Parkway, 89512 Reno, NV, USA
[10]School of Geography, The University of Melbourne, 3010 Victoria, Australia
[11]Institute of Human Origins, Arizona State University, P.O. Box 874101, 85287 Tempe, AZ, USA
[12]Institute of Sciences, Hebrew University of Jerusalem, Edmond J. Safra Campus, Givat Ram, 91904 Jerusalem, Israel
[13]Geological Survey of Israel, 30 Malkhe Israel, 95501 Jerusalem, Israel
[14]MESA Research Unit, Department of Geology, the Faculty of Science, Chulalongkorn University, 10330 Bangkok, Thailand
[15]Institute of Geology and Geophysics, Chinese Academy of Sciences, University of Chinese Academy of Sciences, No. 19 Beitucheng West Road, Chaoyang District, Beijing, China
[16]Institute for Geological and Geochemical Research, Research Centre for Astronomy and Earth Sciences, Hungarian Academy of Sciences, Budaörsi út 45, 1112 Budapest, Hungary
[17]Department of Earth Sciences, University of Southern California, 3651 Trousdale Parkway, 90089 Los Angeles, CA, USA
[18]Institute of Geography, University of Bremen, Bremen, Germany
[19]Dept. of Geoscience, University of Nevada, Box 4010, 89154 Las Vegas, NV, USA
[20]Climate, Atmosphere and Hazards Centre, National Institute of Water & Atmospheric Research, 41 Market Place, Central Business District, Auckland, New Zealand
[21]Department of Geoenvironmental Processes and Global Change, Pyrenean Institute of Ecology (IPE-CSIC), Avda. Montañana 1005, 50059 Zaragoza, Spain
[22]Department of Geological Sciences, Human Evolutionary Research Institute, University of Cape Town, 7701 Rondebosch, Cape Town, South Africa
[23]Department of Geosciences, University of Massachusetts Amherst, 611 North Pleasant Street, 01003-9297 Amherst, MA, USA
[24]Department of Geography, Faculty of Natural Sciences, Jamia Millia Islamia, New Delhi 110025, India

*A full list of authors and their affiliations appears at the end of the paper.

Correspondence: Laia Comas-Bru (laia.comas-bru@ucdconnect.ie)

Received: 13 February 2018 – Discussion started: 16 April 2018
Revised: 13 July 2018 – Accepted: 21 August 2018 – Published: 14 September 2018

Abstract. Stable isotope records from speleothems provide information on past climate changes, most particularly information that can be used to reconstruct past changes in precipitation and atmospheric circulation. These records are increasingly being used to provide "out-of-sample" evaluations of isotope-enabled climate models. SISAL (Speleothem Isotope Synthesis and Analysis) is an international working group of the Past Global Changes (PAGES) project. The working group aims to provide a comprehensive compilation of speleothem isotope records for climate reconstruction and model evaluation. The SISAL database contains data for individual speleothems, grouped by cave system. Stable isotopes of oxygen and carbon ($\delta^{18}O$, $\delta^{13}C$) measurements are referenced by distance from the top or bottom of the speleothem. Additional tables provide information on dating, including information on the dates used to construct the original age model and sufficient information to assess the quality of each data set and to erect a standardized chronology across different speleothems. The metadata table provides location information, information on the full range of measurements carried out on each speleothem and information on the cave system that is relevant to the interpretation of the records, as well as citations for both publications and archived data. The compiled data are available at https://doi.org/10.17864/1947.147.

Geophysical Research Abstracts
Vol. 20, EGU2018-16650, 2018
EGU General Assembly 2018

Preliminary results of the SISAL database

Laia Comas-Bru (1), Sahar Amirnejad (1), Sandy Harrison (2,3), and the SISAL members

(1) University College Dublin, UCD School of Earth Sciences, Dublin, Ireland (laia.comasbru@ucd.ie), (2) School of Archaeology, Geography and Environmental Sciences, University of Reading, Whiteknights, PO Box 227, Reading RG6 6AB, United Kingdom., (3) Centre for Past Climate Change. University of Reading, Whiteknights, PO Box 227, Reading RG6 6AB, United Kingdom.

Speleothems (cave carbonates) provide highly resolved records with the potential to reconstruct past changes in mean regional climate and climate variability on annual to millennial timescales. Some climate models now explicitly include isotopic tracers, and thus the isotopic records from speleothems can be used directly for model evaluation. There are 500+ published speleothem records covering part or all of the last 21,000 years and beyond. However, only 7 speleothems are included in the standard Paleoclimate Modelling Intercomparison Project (PMIP) benchmark dataset.

To address this issue, the SISAL (Speleothem Isotopes Synthesis and Analysis) PAGES working group is creating a data synthesis product compiling the 500+ speleothem records available globally. Such a database (the first for speleothems) can also be used to refine our understanding of regional changes in climate forcings through time, which is crucial in model evaluation. This database, to be published in 2018, will be the first global database of speleothem data containing a comprehensive array of metadata to allow quality control and reliability assessment of the records.

This presentation will showcase the preliminary results of the SISAL database, such as the major changes in isotope signatures for the key periods included in the CMIP6/PMIP4 simulations (Last Glacial Maximum (21 ka), mid-Holocene (6 ka) and Last Millennium (850-1850 CE)) taking into account estimates of measurement or uncertainty.

Preliminary results of the SISAL database

Laia Comas-Bru [1], Sahar Amirnejad [1], Sandy Harrison [2,3], Nick Scroxton [4], István Gábor Hatvani [5], Zoltán Kern [5], Yuval Burstyn [6] and SISAL members

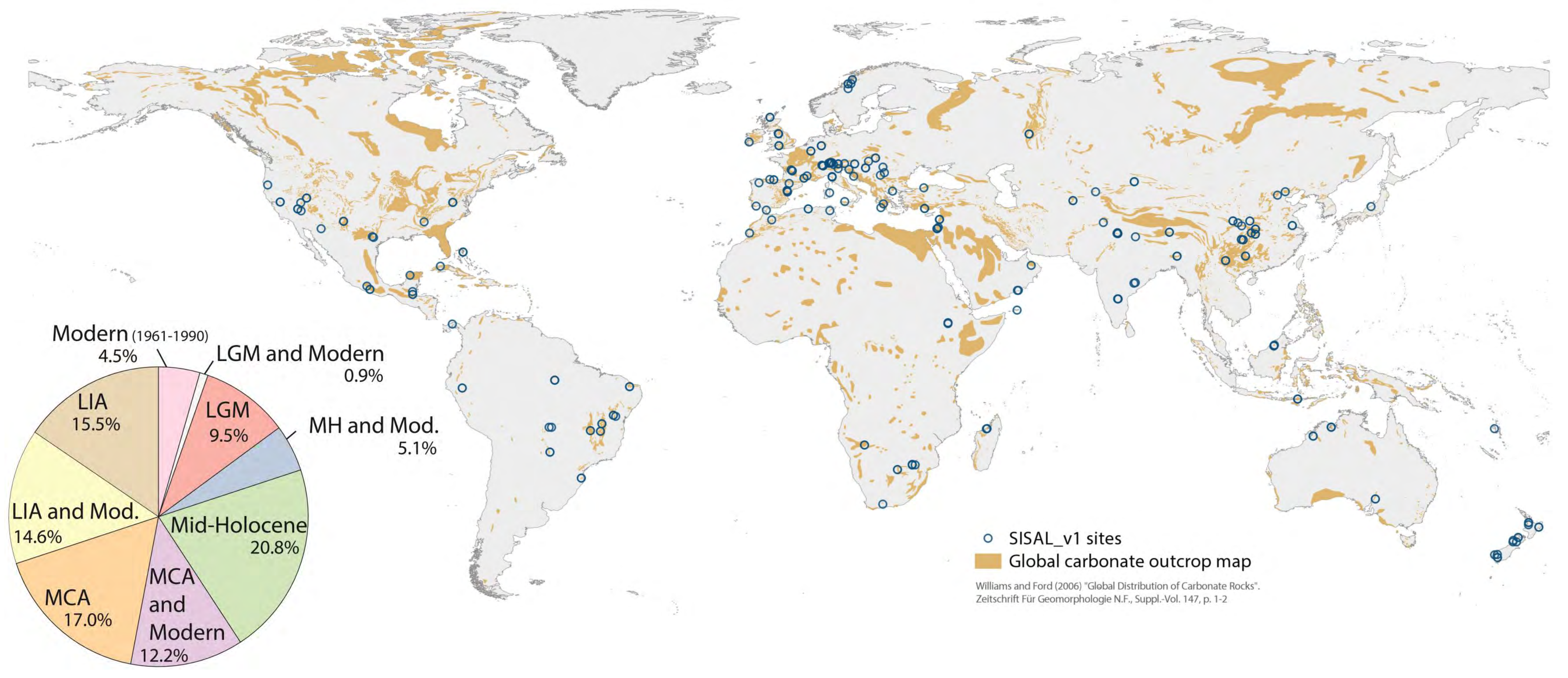
(1) University College Dublin, UCD School of Earth Sciences, Dublin, Ireland (laia.comasbru@ucd.ie)
(2) School of Archaeology, Geography and Environmental Sciences, University of Reading, Whiteknights, PO Box 227, Reading RG6 6AB, United Kingdom.
(3) Centre for Past Climate Change. University of Reading, Whiteknights, PO Box 227, Reading RG6 6AB, United Kingdom.
(4) Department of Geosciences, University of Massachusetts Amherst, MA 01003-9297, United States.
(5) Institute for Geological and Geochemical Research, Research Centre for Astronomy and Earth Sciences, Hungarian Academy of Sciences, H-1112 Budapest. Budaörsi ut 45., Hungary.
(6) Institute of Earth Science/Geology, Hebrew University of Jerusalem, Edmond J. Safra campus, Givat Ram, 91904 Jerusalem, Israel and Geological Survey of Israel, 30 Malkhe Israel, Jerusalem, 95501, Israel

Motivation

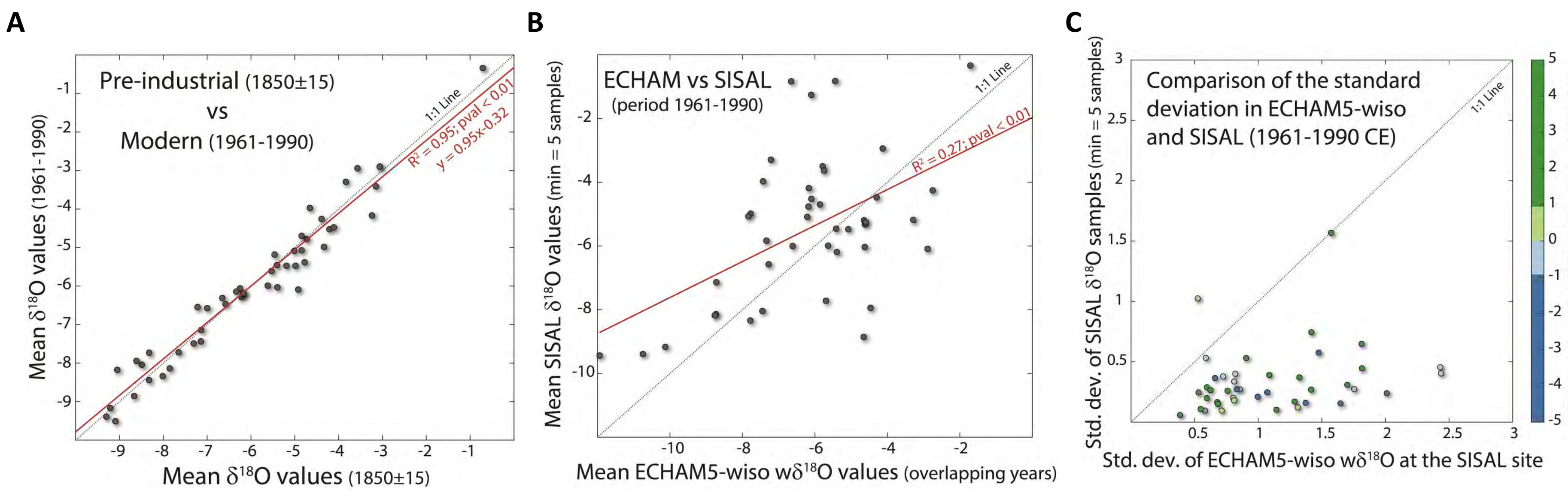
- The SISAL working group is aimed at synthesising and analysing global isotope ($\delta^{18}O$ and $\delta^{13}C$) speleothem data.
- An increasing number of climate models explicitly simulate water isotopes as a tool for characterising and diagnosing the atmospheric hydrological cycle (Schmidt et al., 2007; Werner et al., 2011). Here we show preliminary results using the first version of the SISAL database with the purpose of evaluating such models.
- Comparisons between SISAL data and pollen-based qualitative reconstructions as well as some regional analyses are also presented.

Temporal and spatial coverage

- This map shows the location of SISAL records on a global carbonate outcrop map (Williams and Ford, 2006) to identify potential regions for future speleothem data collection.
- The pie chart shows the percentage of overlap of SISAL records for several key periods (i.e. LIA, MCA, MH and LGM) with modern (1061-1990).



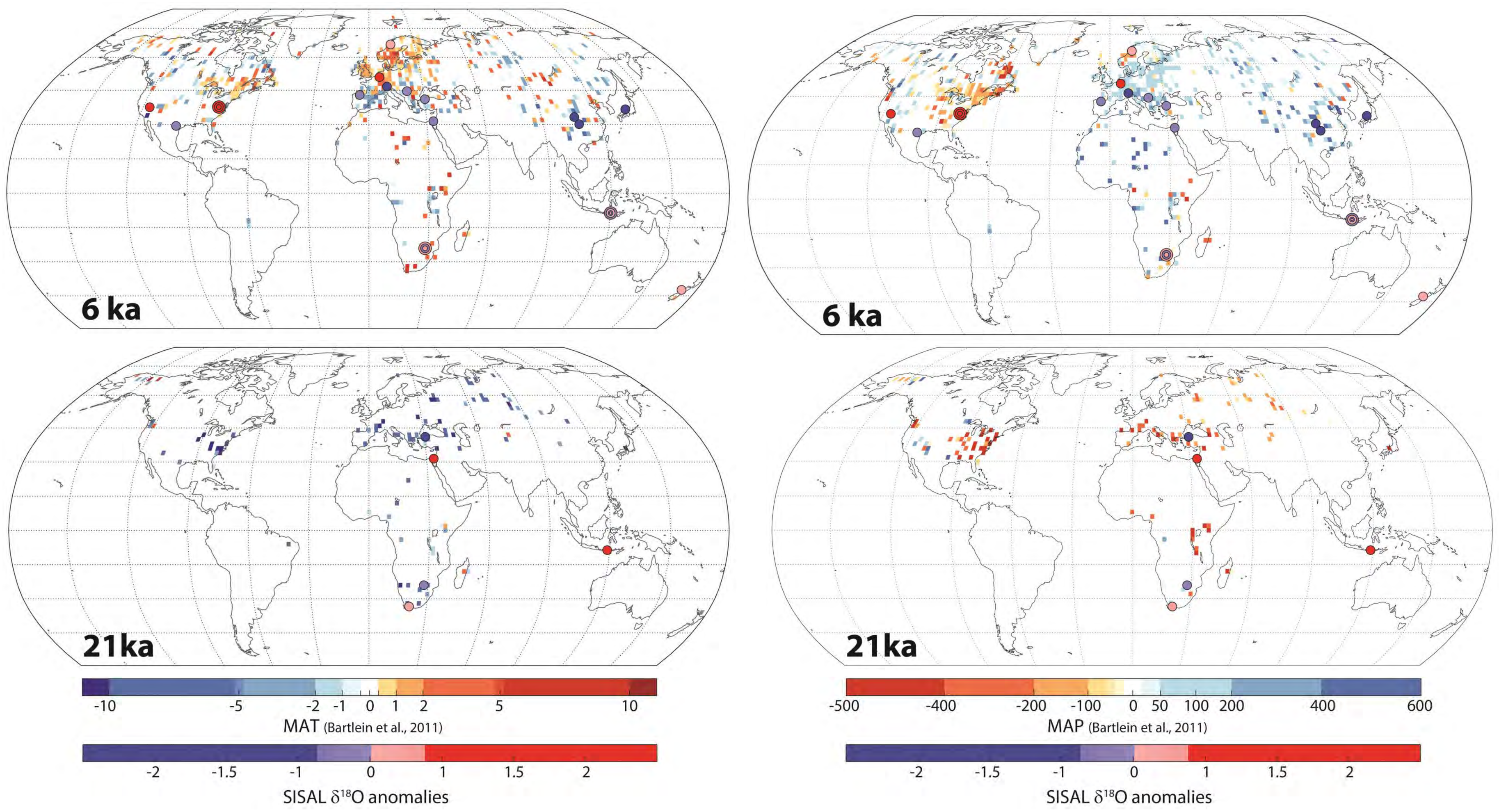
Modern SISAL and ECHAM5-wiso



- The PI is commonly used as reference period by climate models. Its high correlation with the modern period (1961-1990; panel A) indicates the potential suitability of using the latter as a reference to calculate isotope anomalies from SISAL records covering other key periods.
- This results also allows us to use the modern ECHAM5-wiso runs (1958-2013; Werner et al., 2011) to investigate the similarities between SISAL and the isotope-enabled model for the overlapping period. However, the non-significant correlation found (panel B) demonstrates the need to identify a suitable alternative reference period.
- The low variability observed in SISAL compared to that of ECHAM5-wiso data (panel C) is due to the main controls of the speleothem isotope signal (i.e. variable water transit time and in-cave fractionation).

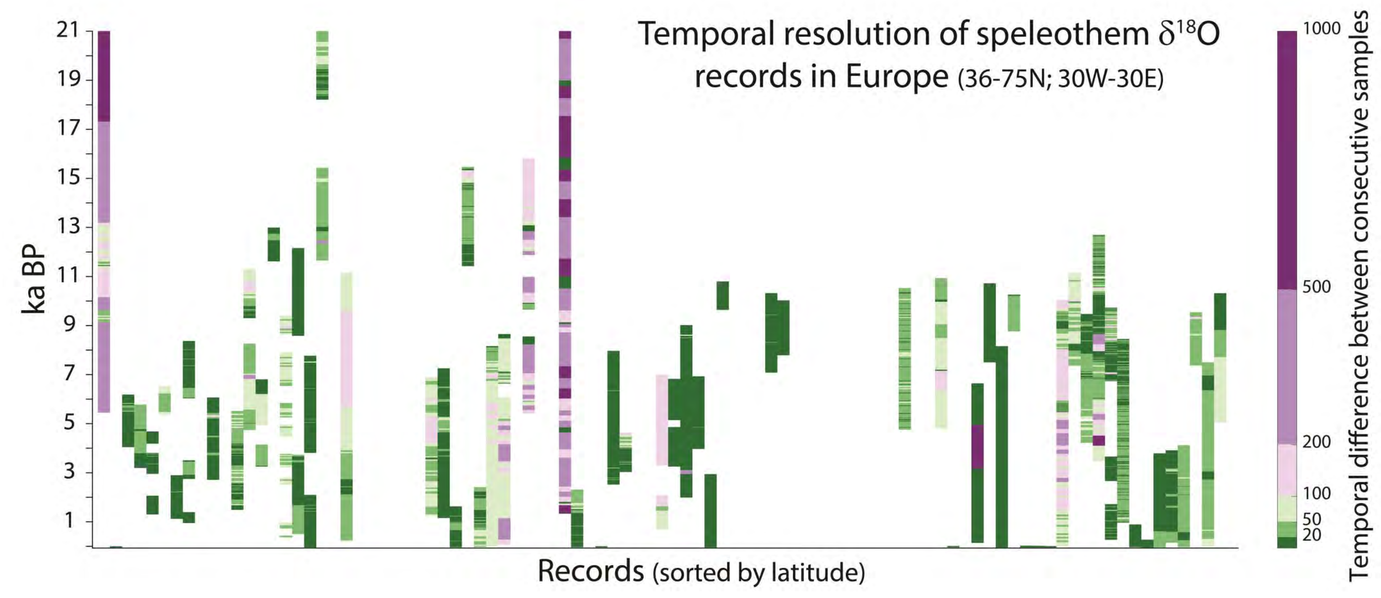
Comparison of SISAL with other palaeoclimate data

- Paleoclimate data of the LGM (21ka) is necessary for data-model comparisons because it allows the evaluation of models with a similar forcing than projected for the next century, while reconstructions of the MH (6ka) provide an opportunity to evaluate the model performance at a time of radically changed seasonality (Schmidt et al., 2014).
- Below we compare SISAL data with a pollen-based qualitative reconstruction of mean annual temperature (MAT; left) and mean annual precipitation (MAP; right) for these two key periods (Bartlein et al., 2011).

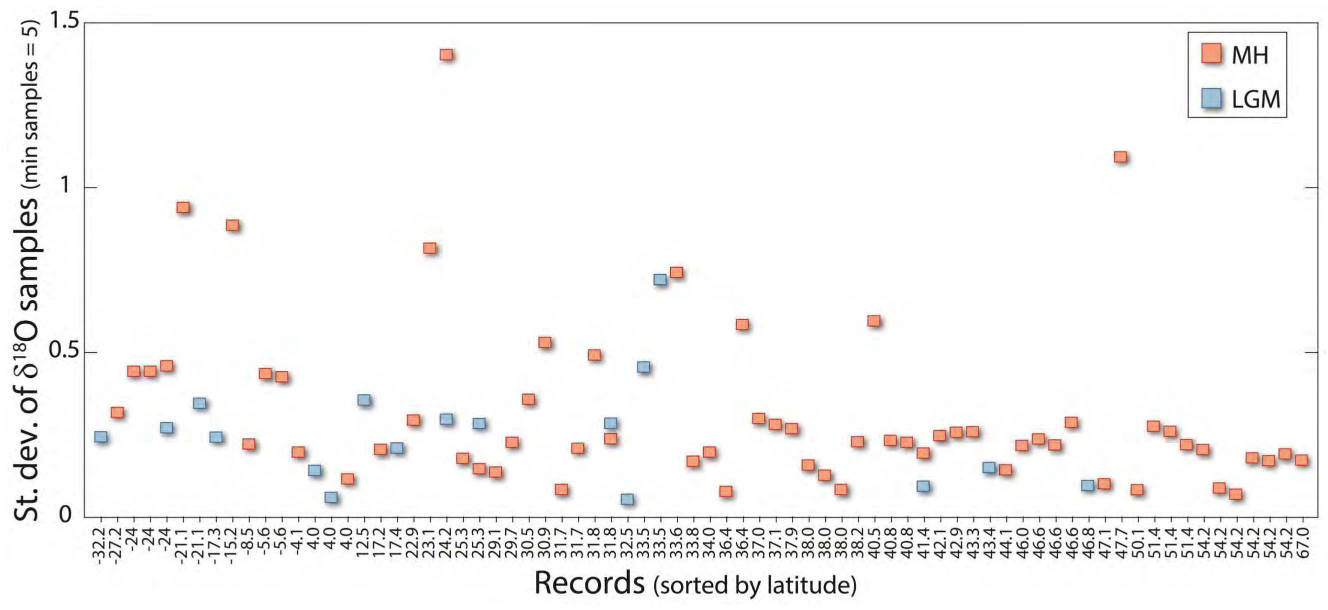


- Overall, reconstructed warm/wet climates correspond with higher isotope anomalies.
- The low number of SISAL sites (circles) are due to the use of the 1961-1990 reference period to calculate the isotope anomalies. This approach significantly constraints the availability of records that cover either LGM-modern or MH-modern (see pie chart above). Future efforts will be focused on identifying a more suitable reference period.

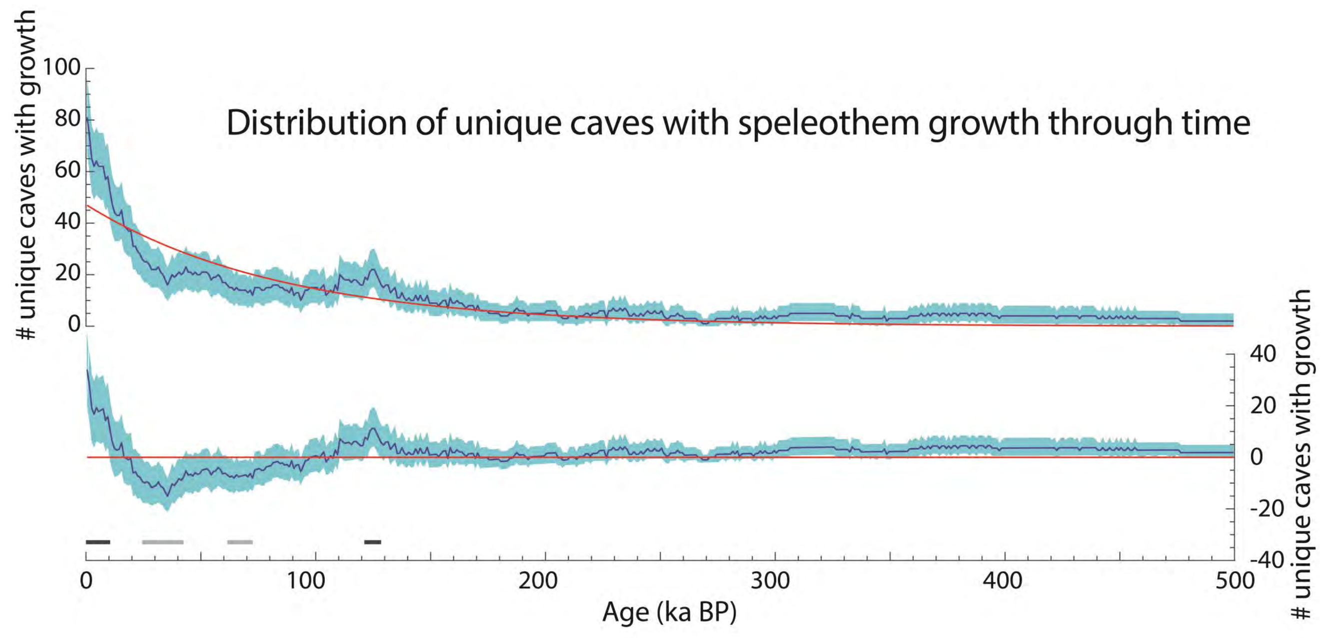
Applications of SISAL



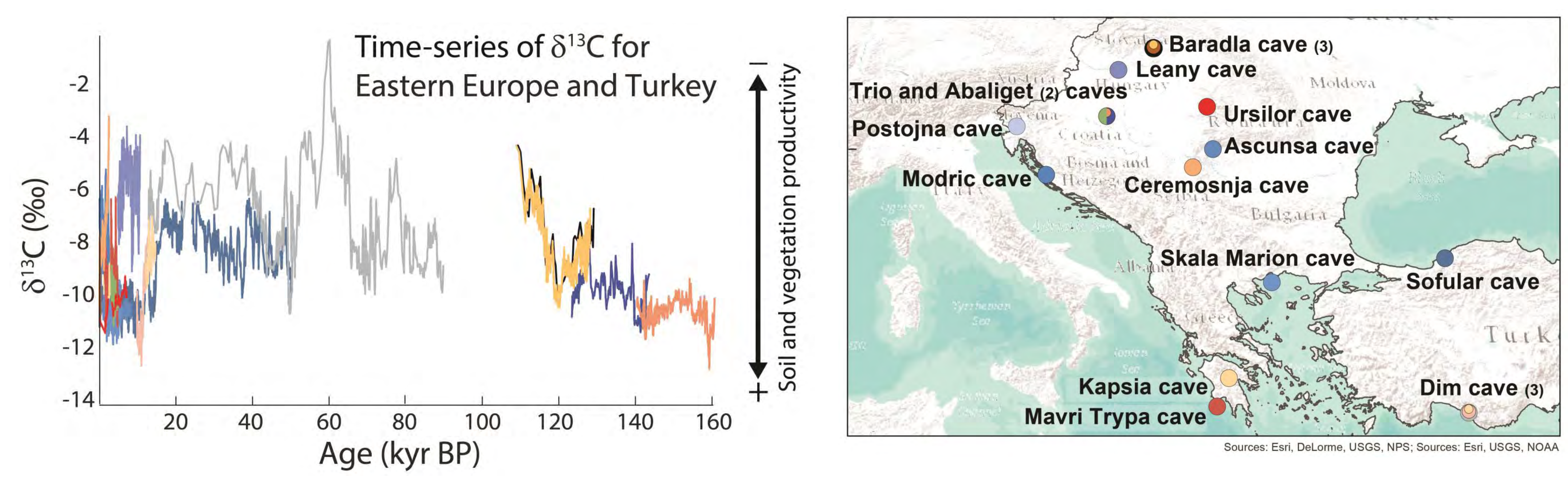
- The figure above shows the temporal distance between isotope samples for all the European records in SISAL. Each bar represents a different speleothem record.
- Most resolutions are between 1 and 100 years, with only 4 records showing millennial scale resolutions. This shows the potential of European records to be used for evaluation of transient model runs.



- Variability of speleothem $\delta^{18}O$ during the MH (6ka ± 150 years) and the LGM (21 ka ± 150 years) is shown here.
- In contrast to recent studies (Rehfeld et al., 2018), our results show a higher inter-annual variability in the warmer MH compared to the LGM.



- The presence, absence and frequency of speleothem growth has been used as a paleoclimate proxy, where wetter conditions generally lead to greater numbers of speleothems (Gascoyne et al., 1983; Vaks et al., 2003).
- Here we show that the total number of unique cave sites with growth approximates an exponential curve (top panel). Deviations from the curve indicate periods of unusually high or low numbers of published speleothem records (bottom panel). This could be due to an abundance/scarcity of growth, a human bias towards/against publishing certain time periods, or both. Periods of anomalously high speleothem growth include interglacials MIS 1 and 5e (dark grey bars), while glacials MIS 2 and 4 (light grey bars) contain fewer than expected records.



- The figure above shows the changes of $\delta^{13}C$ values (19 records) over the last 160 ka for the Eastern Europe-Turkey SISAL Region. It illustrates the increased soil and vegetation productivity during the interglacial/interstadial conditions (mirrored in low $\delta^{13}C$ values). In contrast, in periods with high $\delta^{13}C$, reduced soil and vegetation productivity and relatively increased carbon contribution from the host-rock can be inferred.
- Regional data gives a more comprehensive picture on the region's soil and vegetation productivity changes and infiltration dynamics driven by large scale climate changes compared to single cave studies..

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Geological Survey Suirbhéireacht Gheolaíochta Ireland | Éireann
Roinn Cumarsáide, Gníomhaithe ar son na hAeráide & Comhshaoil
Department of Communications, Climate Action & Environment
PAGES PAST GLOBAL CHANGES

Preliminary results of the SISAL database

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(1) University College Dublin, UCD School of Earth Sciences, Dublin, Ireland (laia.comasbru@ucd.ie)
(2) School of Archaeology, Geography and Environmental Sciences, University of Reading, Whiteknights, PO Box 227, Reading RG6 6AB, United Kingdom.
(3) Centre for Past Climate Change. University of Reading, Whiteknights, PO Box 227, Reading RG6 6AB, United Kingdom.
(4) Alfred Wegener Insitute. Helmholtz Centre for Polar and Marine Research. Division Climate Science – Paleoclimate Dynamics. Bussestr. 24, D-27570 Bremerhaven, Germany
(5) Department of Geosciences, University of Massachusetts Amherst, MA 01003-9297, United States.

SISAL SPELEOTHEM ISOTOPES SYNTHESIS & ANALYSIS

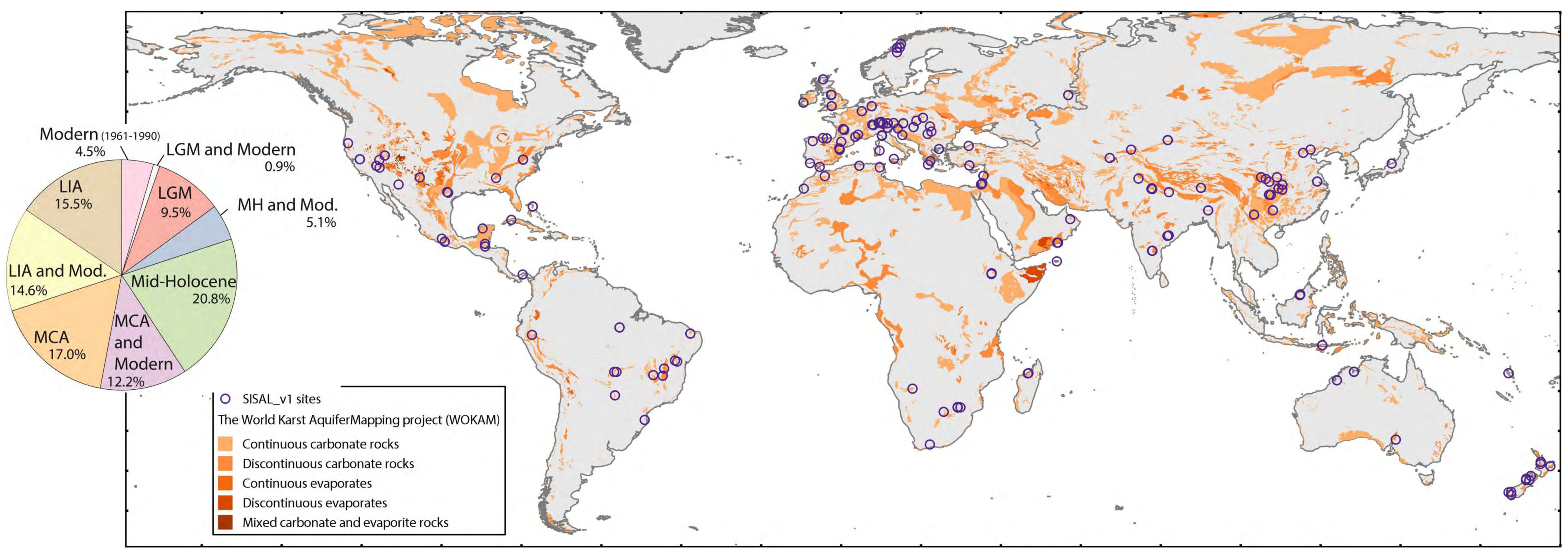
PAGES PAST GLOBAL CHANGES

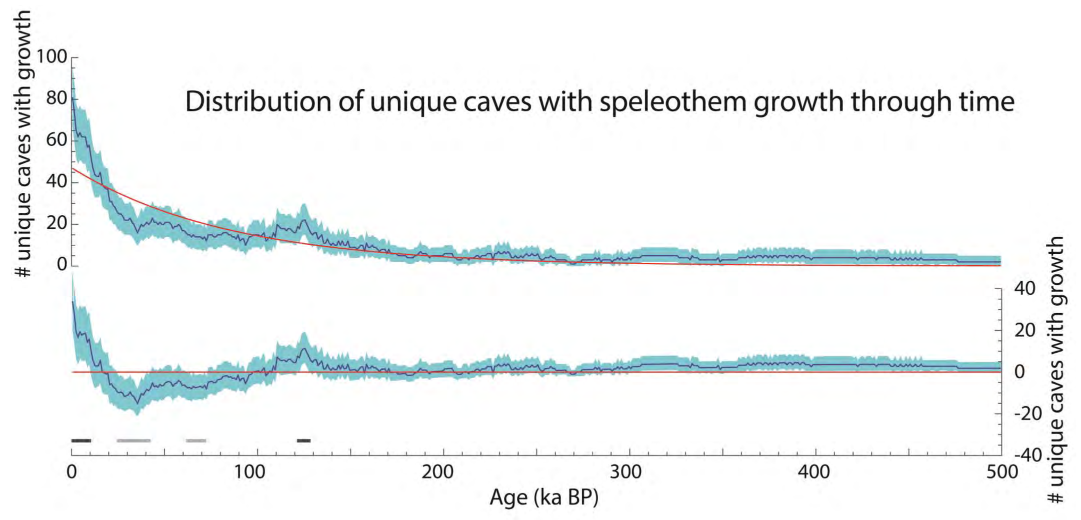
Motivation

- The SISAL working group is aimed at synthesising and analysing global isotope ($\delta^{18}O$ and $\delta^{13}C$) speleothem data.
- An increasing number of climate models explicitly simulate water isotopes as a tool for characterising and diagnosing the atmospheric hydrological cycle (Schmidt et al., 2007; Werner et al., 2011). Here we show preliminary results using the first version of the SISAL database with the purpose of evaluating such models.
- Comparisons between SISAL data and pollen-based qualitative reconstructions as well as some regional analyses are also presented.

Temporal and spatial coverage

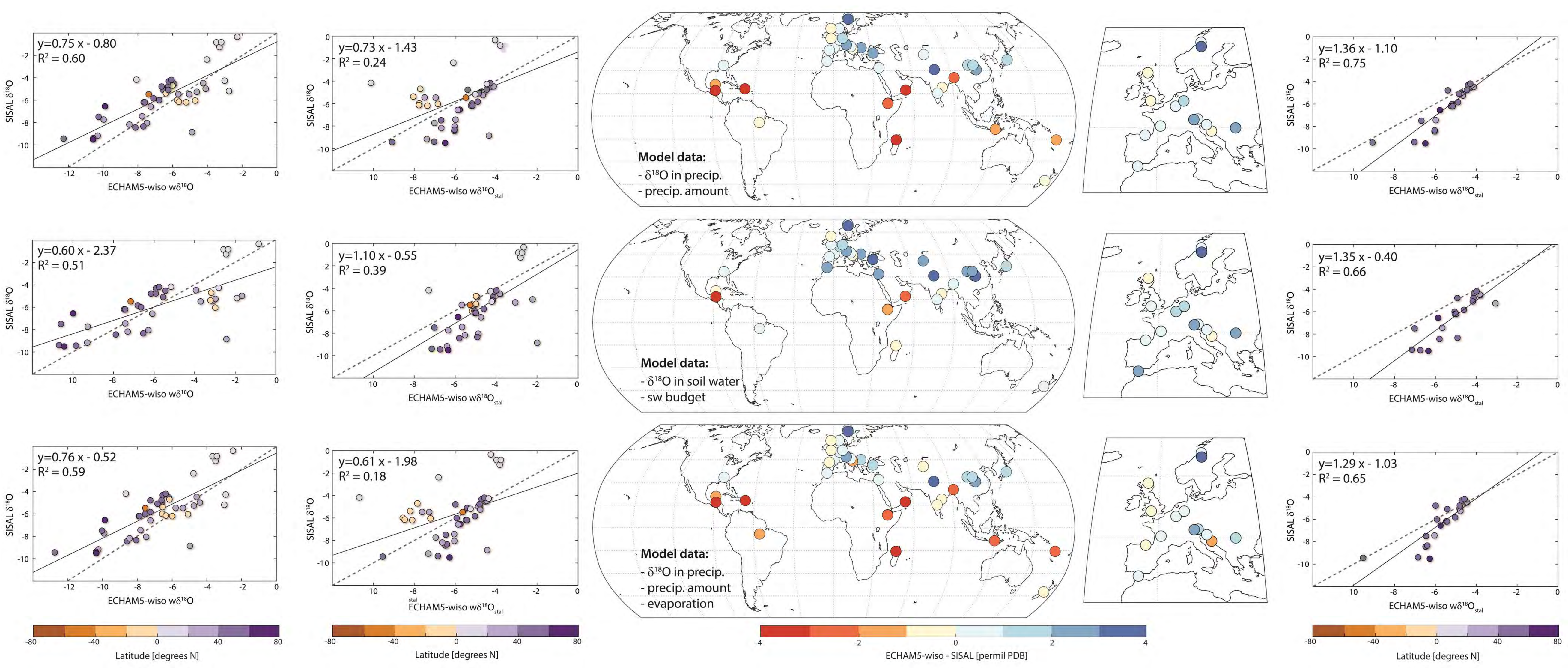
- This map shows the location of SISAL records on a global carbonate outcrop map (WOKAM group) to identify potential regions for future speleothem data collection.
- The pie chart shows the percentage of overlap of SISAL records for several key periods (i.e. LIA, MCA, MH and LGM) with modern (1061-1990).



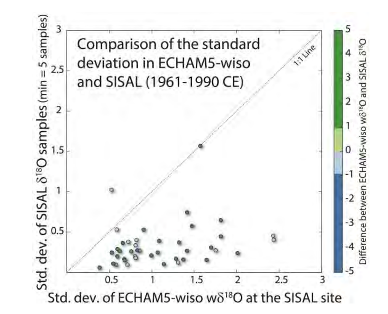


- The presence, absence and frequency of speleothem growth has been used as a paleoclimate proxy, where wetter conditions generally lead to greater numbers of speleothems (Gascoyne et al., 1983; Vaks et al., 2003).
- Here we show that the total number of unique cave sites with growth approximates an exponential curve (top panel). Deviations from the curve indicate periods of unusually high or low numbers of published speleothem records (bottom panel). This could be due to an abundance/scarcity of growth, a human bias towards/against publishing certain time periods, or both. Periods of anomalously high speleothem growth include interglacials MIS 1 and 5e (dark grey bars), while glacials MIS 2 and 4 (light grey bars) contain fewer than expected records.

Modern SISAL and ECHAM5-wiso

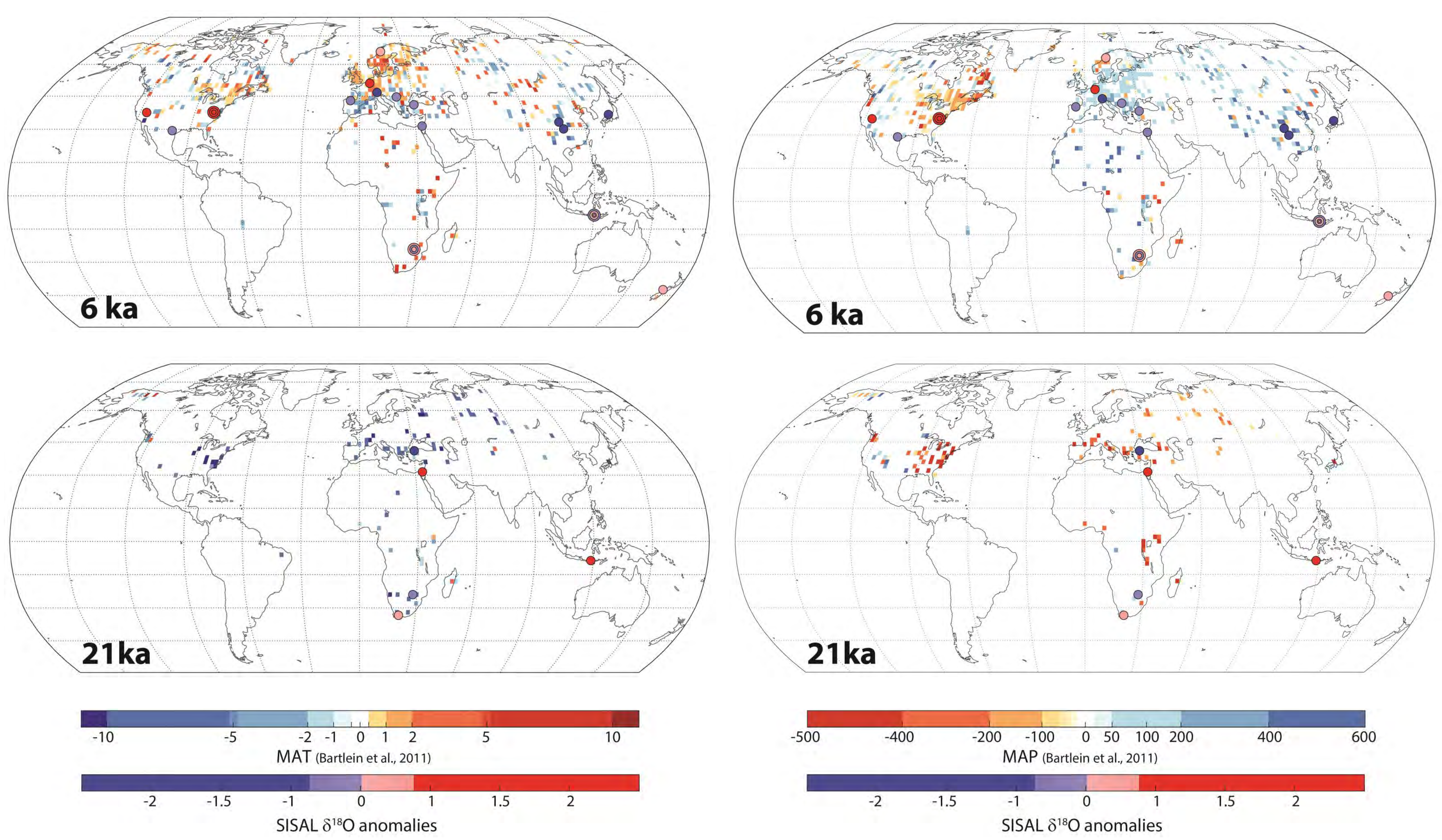


- The PI is commonly used as reference period by climate models. The modern period (1961-1990) in SISAL data is highly correlated with PI (R^2=0.95), indicating its suitability to be used as a reference to calculate isotope anomalies from SISAL records covering other key periods.
- Here we compare the modern ECHAM5-wiso runs (1958-2013; Werner et al., 2011) to investigate the similarities between SISAL and the isotope-enabled model for the 1961-1990 period.
- Three methods are used: weighted $\delta^{18}O$ in precipitation (top); weighted soil water $\delta^{18}O$ (middle); and weighted $\delta^{18}O$ in effective recharge (bottom).
- Due to the dense availability of SISAL records in Europe, the global correlations between SISAL and ECHAM5-wiso are biased towards the correlations found in this region.
- The low variability observed in SISAL compared to that of ECHAM5-wiso data (right) is due to the main controls of the speleothem isotope signal (i.e. variable water transit time and in-cave fractionation).



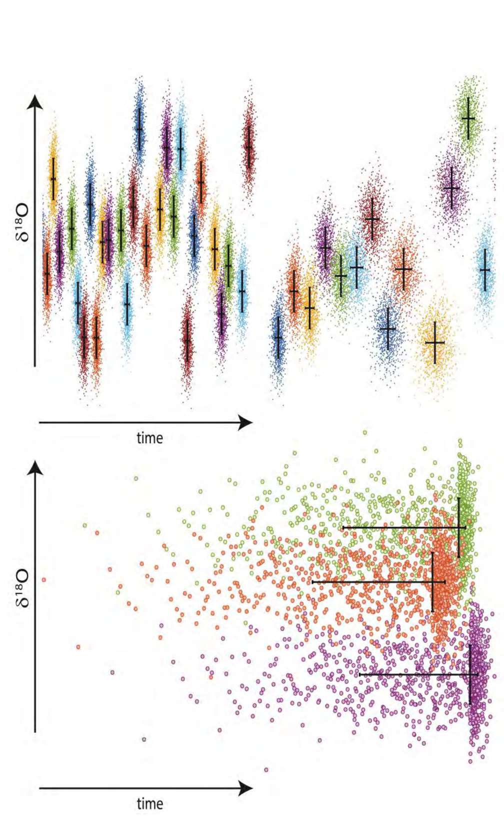
Comparison of SISAL with other palaeoclimate data

- Paleoclimate data of the LGM (21ka) is necessary for data-model comparisons because it allows the evaluation of models with a similar forcing to projected for the next century, while reconstructions of the MH (6ka) provide an opportunity to evaluate the model performance at a time of radically changed seasonality (Schmidt et al., 2014).
- Below we compare SISAL data with a pollen-based qualitative reconstruction of mean annual temperature (MAT; left) and mean annual precipitation (MAP; right) for these two key periods (Bartlein et al., 2011).



- Overall, reconstructed warm/wet climates correspond with higher isotope anomalies.
- The low number of SISAL sites (circles) are due to the use of the 1961-1990 reference period to calculate the isotope anomalies. This approach significantly constraints the availability of records that cover either LGM-modern or MH-modern (see pie chart above). Future efforts will be focused on identifying a more suitable reference period.

Incorporating uncertainties in paleorecords from speleothems



Objective:

Designing a computational toolkit to facilitate the incorporation of uncertainties in paleoclimate variability studies. This toolkit replaces each sample with several isotope-age pairs, representing the same distribution parameters as the original sample.

- For each $\delta^{18}O$ measurement and its corresponding interpolated age, a double Gaussian distribution is generated, using numerous iterations from a bivariate normal random number generator. The mean and covariance matrix are calculated using $\delta^{18}O$ and age values and uncertainties. Correlation coefficient is assumed to be 0
- Observations with asymmetric age uncertainty were assumed to have a dimidated (or bifurcated) Gaussian distribution (Barlow 2003)
- Expectedly distributions for observations with highly asymmetric age uncertainty fail the Lilliefors normality test at 5% significance level
- The large number of isotope-age pairs replacing each sample can bias the results and/or confidence levels of more sophisticated statistical analysis

Future steps

- While in simpler age-modelling methods it can be safely assumed that $\delta^{18}O$ and interpolated age change independently, this would not be accurate for more sophisticated age models and a more realistic estimate of correlation coefficient is required.
- Removing effect of inter-sample dependence, using auto-correlation in order to calculate degree of freedom and assign weights based on DOF (challenge: non-uniform time steps of isotope records)
- Remove effect of spatial dependency, using cross-correlation or variogram to assign weights to different neighbouring records (challenge: poor spatial resolution of records in some areas)

References

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RIA ROYAL IRISH ACADEMY
UCD DUBLIN
Geological Survey Suirbhéireacht Gheolaíochta Ireland | Éireann
Roinn Cumarsáide, Gníomhaithe ar son na hAeráide & Comhshaoil
Department of Communications, Climate Action & Environment