# Towards the construction of regional marine radiocarbon calibration curves: an unsupervised machine learning approach

Ana C. Marza[1], L. Menviel[2], Luke C. Skinner[1]

[1]Department of Earth Sciences, University of Cambridge, Cambridge, CB2 3EQ, United Kingdom
[2]University of New South Wales, Sydney, AUS, Australia

*Correspondence to*: Luke C. Skinner (lcs32@cam.ac.uk)

**SUPPLEMENTARY MATERIAL**

Table S1 summarises the most important software packages used in our analysis. The scripts and complete python environment specifications are hosted at: https://gitlab.com/earth15/ocean_data_clusters.

*Table S1: Principal python packages used.*

| **Package name** | **Version** | **Usage** | **Reference** |
|---|---|---|---|
| *python* | 3.9.14 | Main scripting language | ("The Python Language Reference — Python 3.9.14 Documentation") |
| *numpy* | 1.22.4 | Data manipulation | Harris et al. (2020) |
| *matplotlib* | 3.5.3 | Data visualisation | Hunter (2007) |
| *nctoolkit* | 0.8.4 | NetCDF file manipulation, spatiotemporal statistics | https://nctoolkit.readthedocs.io/en/latest/info.html |
| *sktime* | 0.14.0 | Time series K-Medoids | Löning et al. (2019) |
| *tslearn* | 0.5.2 | Time series K-Means, time series normalisation | Tavenard et al. (2020) |
| *kneed* | 0.8.2 | Locating the elbow point in a plot | https://kneed.readthedocs.io/en/stable/index.html |
| *scipy* | 1.9.3 | Hierarchical clustering | Virtanen et al. (2020) |
| *xesmf* | 0.6.3 | Regridding (nearest_s2d algorithm) | Zhuang et al. (2022) |

**Figure S1.** *Clustering results using K-medoids on un-normalised data from the CM2Mc interglacial run. As for Figure 5 of the main text, but for K increased to K=9.*

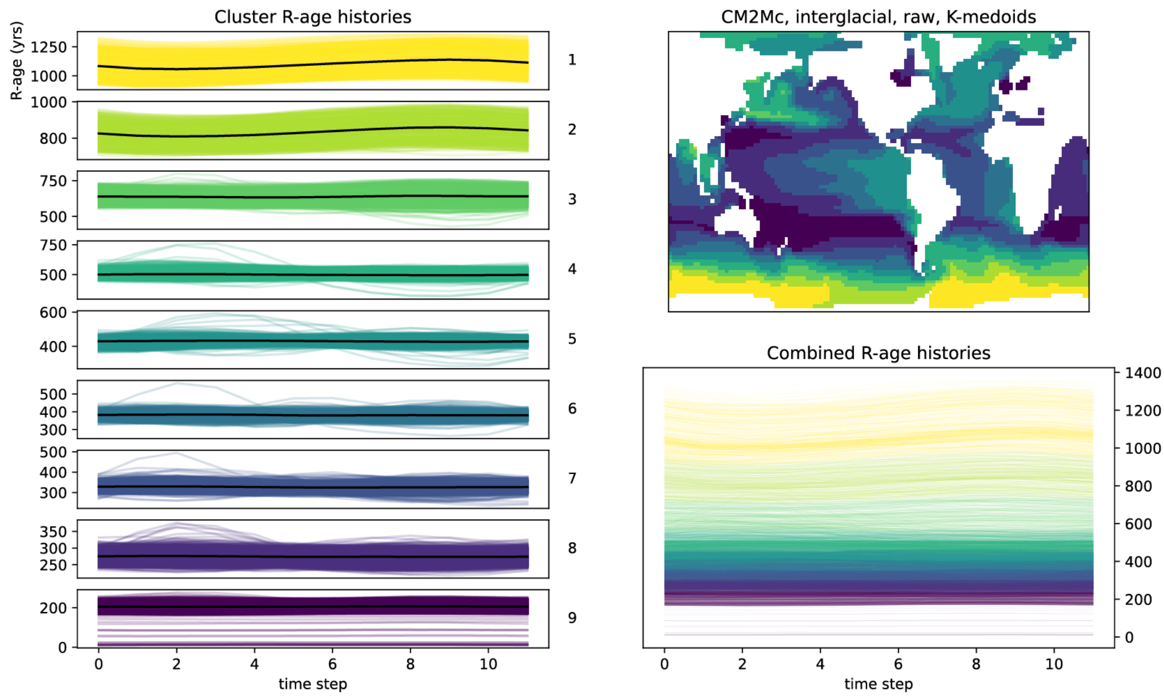


**Figure S2.** *Clustering results using K-Medoids on UVic (U-Tr run) normalised data. As for Figure 9 of the main text, but for K increased to K=8.*

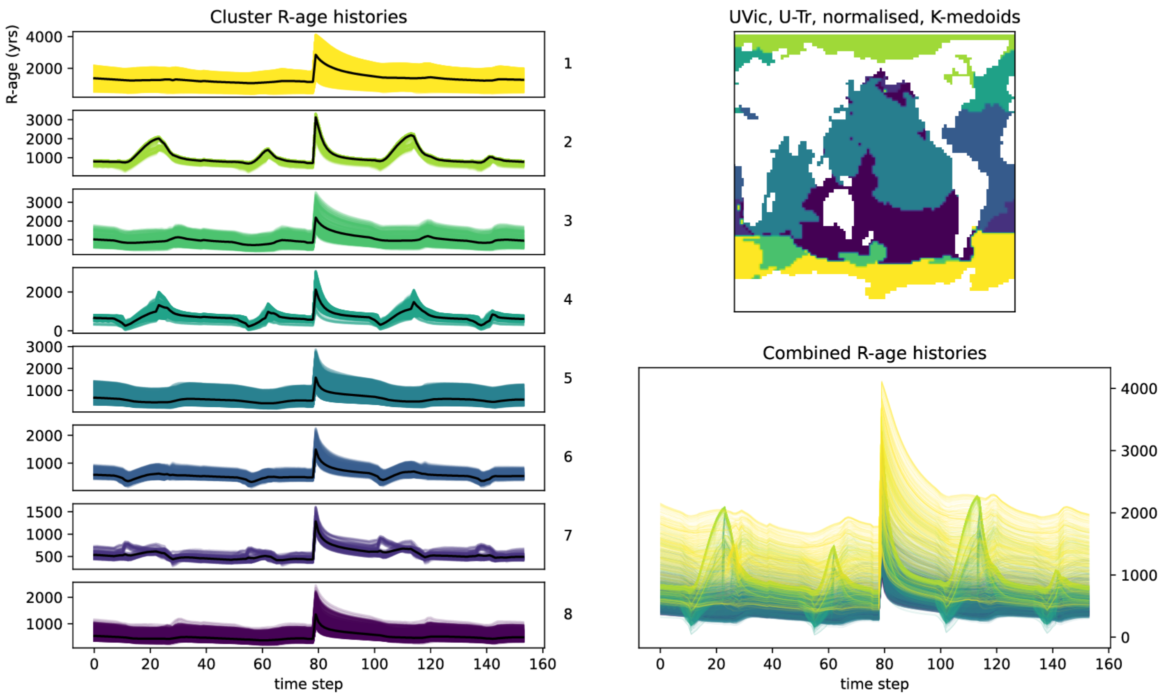


**Figure S3.** *Comparison of clustering results between the UVic U-Tr run (left) and the CM2Mc glacial run (right), using K-medoids on un-normalised data. The colour-coded Venn diagrams quantify overlap between the two maps. Part of the mismatch is attributable to differences in coastal boundaries and model resolutions (here UVic results are re-gridded to permit comparison to CM2Mc).*

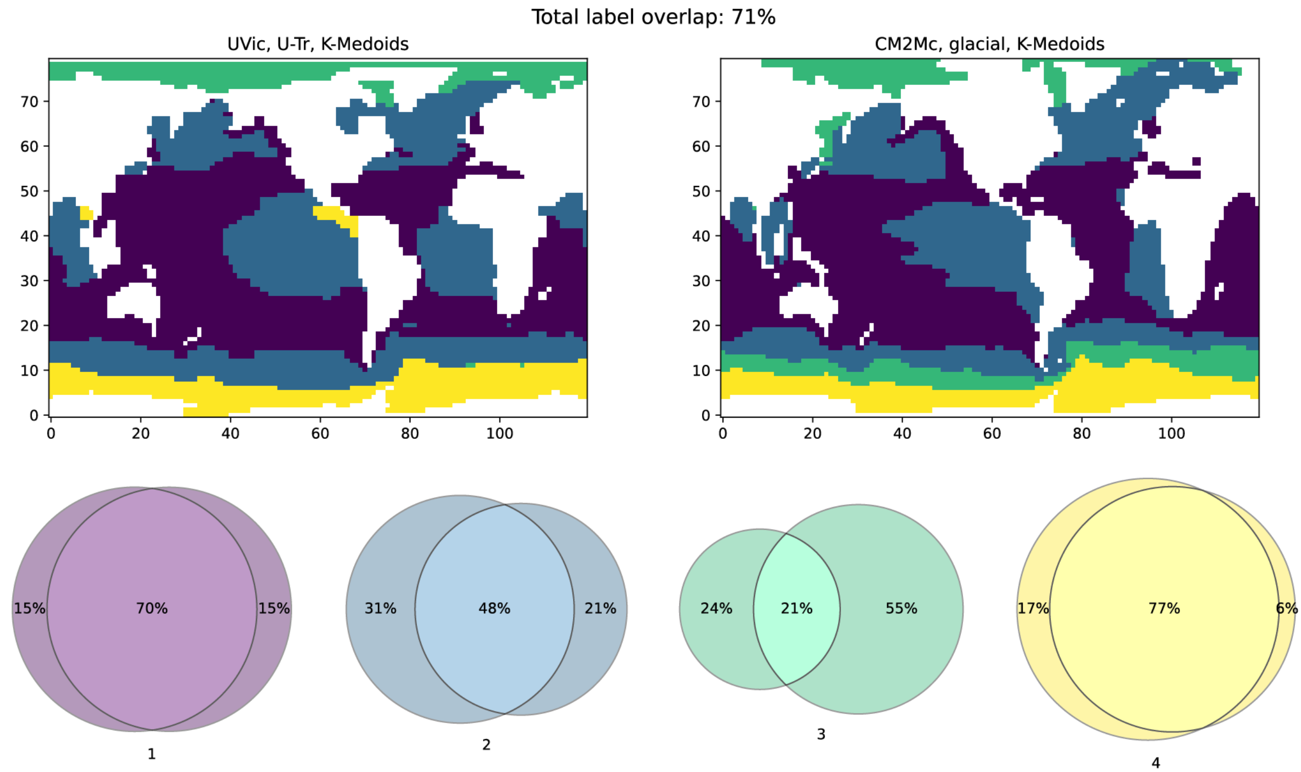
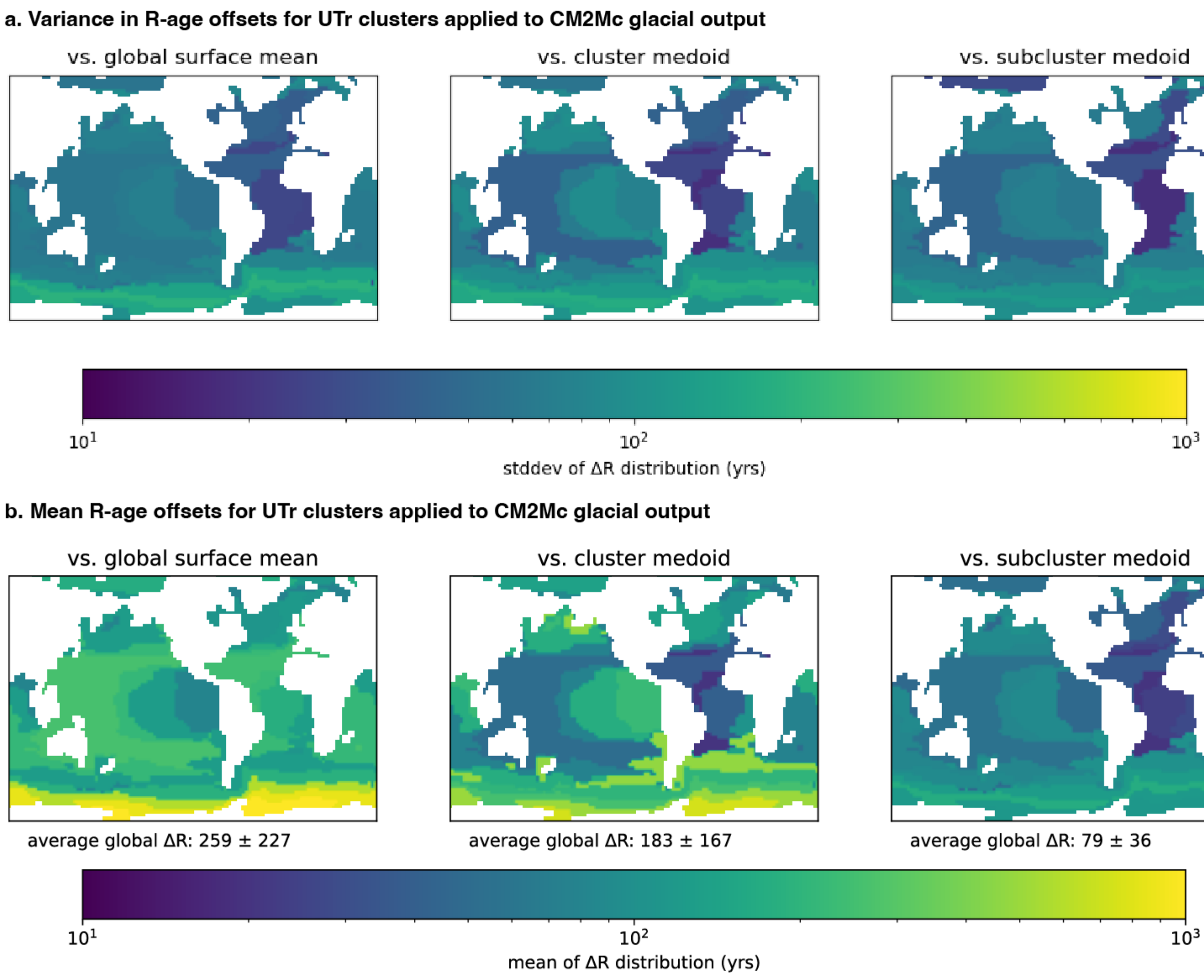


**Figure S4.** *The variance (a.) and mean (b.) of the distribution of R-age offsets in CM2Mc glacial data, when computed relative to three different references: the running mean of the global surface ocean, analogous to e.g. Marine20 (column 1); the medoid of the shape-based cluster to which the subcluster belongs (column 2); and the subcluster's own medoid (column 3). Crucially, and in contrast to Figure 13 of the main text, the geographic definitions of the clusters and their medoids are derived from a different model run (UVic U-Tr). UVic cluster labels were re-gridded to match the resolution of the CM2Mc data.*



## References


Harris, C. R., Millman, K. J., Walt, S. J. v. d., Gommers, R., Virtanen, P., Cournapeau, D., Wieser, E., Taylor, J., Berg, S., Smith, N. J., Kern, R., Picus, M., Hoyer, S., Kerkwijk, M. H. v., Brett, M., Haldane, A., Río, J. F. d., Wiebe, M., Peterson, P., Gérard-Marchant, P., Sheppard, K., Reddy, T., Weckesser, W., Abbasi, H., Gohlke, C., and Oliphant, T. E.: Array programming with NumPy, Nature, 585, 357–362, 10.1038/s41586-020-2649-2, 2020.

Hunter, J. D.: Matplotlib: A 2D graphics environment, Computing in Science & Engineering, 9, 90–95, 10.1109/MCSE.2007.55, 2007.

Löning, M., Bagnall, A., Ganesh, S., Kazakov, V., Lines, J., and Király, F. J.: sktime: A Unified Interface for Machine Learning with Time Series, 2019.

Tavenard, R., Faouzi, J., Vandewiele, G., Divo, F., Androz, G., Holtz, C., Payne, M., Yurchak, R., Rußwurm, M., Kolar, K., and Woods, E.: Tslearn, A Machine Learning Toolkit for Time Series Data, Journal of Machine Learning Research, 21, 1-6, 2020.

Virtanen, P., Gommers, R., Oliphant, T. E., Haberland, M., Reddy, T., Cournapeau, D., Burovski, E., Peterson, P., Weckesser, W., Bright, J., van der Walt, S. J., Brett, M., Wilson, J., Millman, K. J., Mayorov, N., Nelson, A. R. J., Jones, E., Kern, R., Larson, E., Carey, C. J., Polat, İ., Feng, Y., Moore, E. W., VanderPlas, J., Laxalde, D., Perktold, J., Cimrman, R., Henriksen, I., Quintero, E. A., Harris, C. R., Archibald, A. M., Ribeiro, A. H., Pedregosa, F., van Mulbregt, P., and Contributors, S.: SciPy 1.0: Fundamental Algorithms for Scientific Computing in Python, Nature Methods, 17, 261–272, 10.1038/s41592-019-0686-2, 2020.

Zhuang, J., dussin, r., Huard, D., Bourgault, P., Banihirwe, A., Raynaud, S., Malevich, B., Schupfner, M., Levang, S., Jüling, A., Almansi, M., Filipe, RichardScottOZ, RondeauG, Rasp, S., Stachelek, J., Bell, R., Smith, T. J., and Li, X.: pangeo-data/xESMF: v0.7.0, Zenodo [code], 2022.