# Package 'seasonalclumped'

January 14, 2021

Title Toolbox for Clumped Isotope Seasonality Reconstructions

Version 0.3.2

#### Description

Compiles a set of functions and dummy data that simplify reconstructions of seasonal temperature variability in the geological past from stable isotope and clumped isotope records in sub–annually resolved carbonate archives (e.g. mollusk shells, corals and speleothems). For more information, see de Winter et al., 2020 (Climate of the Past Discussions, <doi:10.5194/cp-2020-118>).

**Imports** ggplot2, gridExtra, TTR, magrittr

License GPL-3

URL https://github.com/nielsjdewinter/seasonalclumped

BugReports https://github.com/nielsjdewinter/seasonalclumped/issues

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binning\_seasonality Function for monthly binning based clumped isotope seasonality reconstruction.

## Description

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Combines records of stable oxygen isotope ratios ( $\delta^{18}O_c$ ) and clumped isotope ratios ( $\Delta_{47}$ ) through subannually resolved carbonate archives (e.g. mollusk shells or corals) to reconstruct monthly variability in temperature and salinity (through the  $\delta^{18}O$  composition of the precipitation fluid), using the monthly binning method detailed in de Winter et al., 2020 (Climate of the Past). binning\_seasonality

## Usage

```
binning_seasonality(
    d180c,
    D47,
    ages,
    SD_d180c = 0.1,
    SD_D47 = 0.04,
    N = 1000,
    binsize = "month",
    d180_fun = "KimONeil97",
    D47_fun = "Bernasconi18",
    export = FALSE
)
```

## Arguments

d180c	Vector containing subannually resolved $\delta^{18}O_c$ data
D47	Vector containing subannually resolved $\Delta_{47}$ data
ages	Vector containing ages for of all samples in years relative to the shell chronology
SD_d180c	Error on the $\delta^{18}O_c$ measurements. Either a single value (constant uncertainty) or a vector of length equal to the period in SST data (365 days by default) contain- ing information about the error of each datapoint (1 standard deviation; default = 0.1 permille).
SD_D47	Error on the $\Delta_{47}$ measurements. Either a single value (constant uncertainty) or a vector of length equal to the period in SST data (365 days by default) containing information about the error of each datapoint (1 standard deviation; default = 0.04 permille).
Ν	Number of datapoints for Monte Carlo simulation (defaults to 1000)
N binsize	Number of datapoints for Monte Carlo simulation (defaults to 1000) Size of the bins in which records are subdivided. month and season (period of three months) is currently supported.
	Size of the bins in which records are subdivided. month and season (period of
binsize	Size of the bins in which records are subdivided. month and season (period of three months) is currently supported. String containing the name of the transfer function used to convert temperature and $\delta^{18}O_w$ to $\delta^{18}O_c$ data (for example: "KimONei197" or "GrossmanKu86").

## Value

A data frame containing monthly reconstructions of  $\Delta_{47}$ , temperature,  $\delta^{18}O$  of the precipitation fluid and  $\delta^{18}O_c$ .

#### References

Grossman, E.L., Ku, T., Oxygen and carbon isotope fractionation in biogenic aragonite: temperature effects, *Chemical Geology* **1986**, *59.1*, 59–74. https://doi.org/bvpzws

Kim, S., O'Niel, J.R., Equilibrium and nonequilibrium oxygen isotope effects in synthetic carbonates, *Geochimica et Cosmochimica Acta* **1997**, *61.16*, 3461–3475. https://doi.org/c7bwbp

Dettman, D.L., Reische, A.K., Lohmann, K.C., Controls on the stable isotope composition of seasonal growth bands in aragonitic fresh-water bivalves (Unionidae), *Geochimica et Cosmochimica Acta* **1999**, *63.7–8*, 1049–1057. https://doi.org/cbb7zc

Brand, W.A., Coplen, T.B., Vogl, J., Rosner, M., Prohaska, T., Assessment of international reference materials for isotope–ratio analysis (IUPAC Technical Report), *Pure and Applied Chemistry* **2014**, *86.3*, 425–467. https://doi.org/fpc2

Kele, S., Breitenbach, S. F., Capezzuoli, E., Meckler, A. N., Ziegler, M., Millan, I. M., Kluge, T., Deák, J., Hanselmann, K. and John, C. M., Temperature dependence of oxygen– and clumped isotope fractionation in carbonates: a study of travertines and tufas in the 6–95 C temperature range, *Geochimica et Cosmochimica Acta* **2015**, 168, 172–192. https://doi.org/f7sgn6

Bernasconi, S.M., Müller, I.A., Bergmann, K.D., Breitenbach, S.F., Fernandez, A., Hodell, D.A., Jaggi, M., Meckler, A.N., Millan, I. and Ziegler, M., Reducing uncertainties in carbonate–clumped isotope analysis through consistent carbonate based standardization. *Geochemistry, Geophysics, Geosystems* **2018**, 19–9, 2895–2914. https://doi.org/gfmjrw

Petersen, S. V., Defliese, W. F., Saenger, C., Daëron, M., Huntington, K. W., John, C. M., Kelson, J. R., Bernasconi, S. M., Colman, A. S., Kluge, T., Olack, G. A., Schauer, A. J., Bajnai, D., Bonifacie, M., Breitenbach, S. F. M., Fiebig, J., Fernandez, A. B., Henkes, G. A., Hodell, D., Katz, A., Kele, S., Lohmann, K. C., Passey, B. H., Peral, M. Y., Petrizzo, D. A., Rosenheim, B. E., Tripati, A., Venturelli, R., Young, E. D. and Winkelstern, I. Z., Effects of Improved 17O Correction on Interlaboratory Agreement in Clumped Isotope Calibrations, Estimates of Mineral–Specific Offsets, and Temperature Dependence of Acid Digestion Fractionation, *Geochemistry, Geophysics, Geosystems* \*2019, 20–7, 3495–3519. https://doi.org/ggrc39

Jautzy, J. J., Savard, M. M., Dhillon, R. S., Bernasconi, S. M. and Smirnoff, A., Clumped isotope temperature calibration for calcite: Bridging theory and experimentation, *Geochemical Perspectives Letters* **2020**, 14, 36–41. https://doi.org/fpc3

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

## Examples

```
# find attached dummy data
Case1 <- seasonalclumped::Case1
d180c <- Case1[, 29]
d180c <- d180c[-which(is.na(d180c))]
D47 <- Case1[, 30]
D47 <- D47[-which(is.na(D47))]
ages <- Case1[, 27]
ages <- ages[-which(is.na(ages))]
# Run function
binned <- binning_seasonality(d180c,
D47,
ages,
```

carbmodel

```
0.1,
0.04,
100, # Use small amount of samples for quick testing (recommended N = 1000)
"month",
"KimONei197",
"Bernasconi18",
FALSE)
```

carbmodel

Function that produces  $\delta^{18O}$  and  $\Delta_{47}$  records

## Description

Takes vectors of time, temperature, growth rate and  $\delta^{18}O$  of the fluid and converts them into a  $\delta^{18}O$  and  $\Delta_{47}$  record. The  $\delta^{18}O$  and  $\Delta_{47}$  values are calculated for every depth value provided in the D vector. By default, the empirical transfer function by Kim and O'Neil (1997) is used to produce the  $\delta^{18}O$  record, but other transfer functions (e.g. Grossman and Ku, 1986) are also supported. The default transfer function for converting temperature data to  $\Delta_{47}$  data is based on Bernasconi et al. (2018), but other transfer functions (e.g. Jautzy et al., 2020) are also supported.

## Usage

```
carbmodel(
  time,
  SST,
  GR,
  d180w,
  D,
  d180_fun = "KimONeil97",
  D47_fun = "Bernasconi18",
  AV = FALSE,
  plot = FALSE
)
```

#### Arguments

time	Time vector (values in years)
SST	A vector containing temperature data (values in degrees C; length must be equal to that of time)
GR	Growth rate vector (values in same time unit as time (years); length must be equal to that of time)
d180w	A vector containing data on the $\delta^{18}O$ value of the precipitation fluid (values in permille VSMOW; length must be equal to that of time)
D	Depth vector (values in same depth unit as GR)
d180_fun	String containing the name of the transfer function used to convert temperature and $\delta^{18}O_w$ to $\delta^{18}O_c$ data (for example: "KimONeil97" or "GrossmanKu86"). Defaults to Kim and O'Neil (1997).

D47_fun	String containing the name of the transfer function used to convert temperature to $\Delta_{47}$ data (for example: "Bernasconi18" or "Jautzy20"). Defaults to Bernasconi et al., 2018).
AV	Should the subsampling take into account the mean value within the sample interval? TRUE/FALSE If FALSE, the interpolated value corresponding to the exact position is used instead of the mean of the interval
plot	Should the result be plotted? TRUE/FALSE

## Value

A matrix containing subsampled time, depth,  $\delta^{18}O_c$  and  $\Delta_{47}$  values: "Tnew"): New time vector after subsampling "D"): New depth vector after subsampling "d180c"): Vector listing  $\delta^{18}O_c$  values for each sample "D47"): Vector listing  $\Delta_{47}$  values for each sample

#### References

package dependencies: ggplot2, gridExtra function dependencies: subsample, subsample\_mean Grossman, E.L., Ku, T., Oxygen and carbon isotope fractionation in biogenic aragonite: temperature effects, *Chemical Geology* **1986**, *59.1*, 59–74. https://doi.org/bvpzws

Kim, S., O'Niel, J.R., Equilibrium and nonequilibrium oxygen isotope effects in synthetic carbonates, *Geochimica et Cosmochimica Acta* **1997**, *61.16*, 3461–3475. https://doi.org/c7bwbp

Dettman, D.L., Reische, A.K., Lohmann, K.C., Controls on the stable isotope composition of seasonal growth bands in aragonitic fresh-water bivalves (Unionidae), *Geochimica et Cosmochimica Acta* **1999**, *63.7–8*, 1049–1057. https://doi.org/cbb7zc

Brand, W.A., Coplen, T.B., Vogl, J., Rosner, M., Prohaska, T., Assessment of international reference materials for isotope–ratio analysis (IUPAC Technical Report), *Pure and Applied Chemistry* **2014**, *86.3*, 425–467. https://doi.org/fpc2

Kele, S., Breitenbach, S. F., Capezzuoli, E., Meckler, A. N., Ziegler, M., Millan, I. M., Kluge, T., Deák, J., Hanselmann, K. and John, C. M., Temperature dependence of oxygen– and clumped isotope fractionation in carbonates: a study of travertines and tufas in the 6–95 C temperature range, *Geochimica et Cosmochimica Acta* **2015**, 168, 172–192. https://doi.org/f7sgn6

Bernasconi, S.M., Müller, I.A., Bergmann, K.D., Breitenbach, S.F., Fernandez, A., Hodell, D.A., Jaggi, M., Meckler, A.N., Millan, I. and Ziegler, M., Reducing uncertainties in carbonate–clumped isotope analysis through consistent carbonate based standardization. *Geochemistry, Geophysics, Geosystems* **2018**, 19–9, 2895–2914. https://doi.org/gfmjrw

Petersen, S. V., Defliese, W. F., Saenger, C., Daëron, M., Huntington, K. W., John, C. M., Kelson, J. R., Bernasconi, S. M., Colman, A. S., Kluge, T., Olack, G. A., Schauer, A. J., Bajnai, D., Bonifacie, M., Breitenbach, S. F. M., Fiebig, J., Fernandez, A. B., Henkes, G. A., Hodell, D., Katz, A., Kele, S., Lohmann, K. C., Passey, B. H., Peral, M. Y., Petrizzo, D. A., Rosenheim, B. E., Tripati, A., Venturelli, R., Young, E. D. and Winkelstern, I. Z., Effects of Improved 17O Correction on Interlaboratory Agreement in Clumped Isotope Calibrations, Estimates of Mineral–Specific Offsets, and Temperature Dependence of Acid Digestion Fractionation, *Geochemistry, Geophysics, Geosystems* \*2019, 20–7, 3495–3519. https://doi.org/ggrc39

Jautzy, J. J., Savard, M. M., Dhillon, R. S., Bernasconi, S. M. and Smirnoff, A., Clumped isotope temperature calibration for calcite: Bridging theory and experimentation, *Geochemical Perspectives Letters* **2020**, 14, 36–41. https://doi.org/fpc3

## Examples

```
# Create test data (= ideal case)
# Set boundary conditions
Td <- seq(1, 12 * 365, 1) # Create timeline of 12 years in days
Ty <- Td / 365 # Convert to years
MAT <- 20 # Set mean annual temperature
Amp <- 10 # Set seasonal amplitude
Sext <- 2 * Amp # Calculate extent of seasonal variability</pre>
TSD <- 1.5 # Set the degree of random non–seasonal noise on the SST curve
# ("weather")
SST <- rnorm(length(Ty), MAT + Amp * sin(2 * pi * Ty), TSD) # Create virtual</pre>
# daily SST data
GR <- rep(10 / 365, length(Ty)) # Set growth rate to 10 mm/yr and create daily
# GR vector
DSD <- 0.6 # Set the degree of random non–seasonal noise on the d180sw curve
# ("salinity fluctuations")
d180sw<-rnorm(length(Ty), rep(0, length(Ty)), DSD) # Set d180sw to 0 permille
# VSMOW, create daily d180sw vector
SR <- 0.75 # Set sampling resolution to 0.75 mm
# Create vector for all samples along entire shell length by applying constant
# sampling resolution
D <- seq(SR, sum(GR), SR)</pre>
# Calculate virtual data
newdata <- carbmodel(Ty, SST, GR, d180sw, D, AV = TRUE)</pre>
```

Case1

Virtual dataset Case 1

## Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 1 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case1

#### Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

Tnew Age, in years relative to the start of the record

D Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

- **d18Oc** stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille

SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille ...

## Details

Case 1 describes an ideal temperature sinusoid without distortion by either changes in growth rate or changes in  $\delta^{18}O_w$ .

Generated using the code in "Generate\_Case1.r" in dataraw

#### Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

#### Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 10 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case10

## Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

**D47** clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm
- **Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

#### Details

Case 10 describes an ideal temperature sinusoid without distortion by changes in growth rate, but a negative peak in  $\delta^{18}O_w$  during spring season.

Generated using the code in "Generate\_Case10.r" in dataraw

#### Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

Case11

Virtual dataset Case 11

## Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 11 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case11

## Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

#### Details

Case 11 describes an ideal temperature sinusoid without distortion by changes in growth rate, but a positive peak in  $\delta^{18}O_w$  during the warm season.

Generated using the code in "Generate\_Case11.r" in dataraw

#### Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

Case12

Virtual dataset Case 12

## Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 12 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case12

## Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

D Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

**D47** clumped isotope value, in permille

SR\_ 0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm

Tnew Age, in years relative to the start of the record

- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille ...

## Details

Case 12 describes a temperature sinusoid without distortion by changes in growth rate or  $\delta^{18}O_w$ , but with a multi–annual trend in temperature superimposed on the seasonality.

Generated using the code in "Generate\_Case12.r" in dataraw

## Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

#### Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 13 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case13

## Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

**D47** clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm
- **Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

## Details

Case 13 describes a temperature sinusoid without distortion by changes in growth rate but with a multi–annual trend in  $\delta^{18}O_w$  superimposed on the seasonality.

Generated using the code in "Generate\_Case13.r" in dataraw

#### Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

Case14

Virtual dataset Case 14

## Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 14 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case14

## Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

## Details

Virtual case simulating open marine conditions: Seasonal change in growth rate in phase with temperature with linear growth decrease and dynamic growth threshold. Multi–annual cyclicity in  $\delta^{18}O_w$  (NAO–style).

Generated using the code in "Generate\_Case14.r" in dataraw

#### Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

Example of natural NAO oscillation:

Sarafanov, A., On the effect of the North Atlantic Oscillation on temperature and salinity of the subpolar North Atlantic intermediate and deep waters *ICES Journal of Marine Science* **2009**, *66.7*, 1448–1454. doi: 10.1093/icesjms/fsp094

Case15

Virtual dataset Case 15

## Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 15 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case15

#### Format

A data frame with 1200 rows and 30 variables:

SR\_ 0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

**SR\_0.2** Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

- D47 clumped isotope value, in permille
- SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm
- Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm
- **Tnew** Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille ...

## Details

Case simulating a coastal ecosystem: Seasonal change in growth rate with fast growth in spring and linear growth decrease. Pulse of light  $\delta^{18}O_w$  in spring and multi–annual cyclicity in SST.

Generated using the code in "Generate\_Case15.r" in dataraw

#### Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

#### Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 16 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case16

## Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

**D47** clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm
- Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

#### Details

Case simulating a lagoonal ecosystem – Seasonal change in growth rate with slower growth in summer and linear growth decrease. Pulse of increased  $\delta^{18}O_w$  in summer (evaporation).

Generated using the code in "Generate\_Case16.r" in dataraw

#### Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

Case17

Virtual dataset Case 17

## Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 17 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case17

## Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

## Details

Case simulating a tropical ecosystem – Slight seasonal change in growth rate with slower growth in summer and linear growth decrease. Confined temperature seasonality, relatively strong multi–annual trend. Strong  $\delta^{18}O_w$  seasonality, light in summer, multi–annual trend in antiphase with multi–annual SST (ENSO–style)

Generated using the code in "Generate\_Case17.r" in dataraw

#### Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

Example of modern ENSO variability: Iijima, H., Kayanne, H., Morimoto, M., Abe, O. Interannual sea surface salinity changes in the western Pacific from 1954 to 2000 based on coral isotope analysis, *Geophysical research letters*, **2005**, *32.4*, 1–4. https://doi.org/bhv8dn

Case18

Virtual dataset Case 18

## Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 18 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case18

#### Format

A data frame with 1200 rows and 30 variables:

SR\_ 0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

Tnew Age, in years relative to the start of the record

D Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

**D47** clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

- D47 clumped isotope value, in permille
- SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm
- Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record
- D Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm
- **Tnew** Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille ...

## Details

Case simulating a high-latitude shallow marine ecosystem: Spring freshening and growth only during summer half of season

Generated using the code in "Generate\_Case18.r" in dataraw

## Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

#### Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 19 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case19

## Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

**D47** clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm
- **Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

## Details

Case 19 describes an ideal temperature sinusoid without distortion by either changes in growth rate or changes in  $\delta^{18}O_w$  but with a smaller temperature amplitude.

Generated using the code in "Generate\_Case19.r" in dataraw

#### Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

Case2

Virtual dataset Case 2

## Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 2 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case2

## Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

## Details

Case 2 describes an ideal temperature sinusoid without distortion by changes in  $\delta^{(18)}O_w$ , but with a growth stop in the cold season.

Generated using the code in "Generate\_Case2.r" in dataraw

#### Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

Case20

Virtual dataset Case 20

## Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 20 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case20

## Format

A data frame with 1200 rows and 30 variables:

SR\_ 0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

Tnew Age, in years relative to the start of the record

D Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm

Tnew Age, in years relative to the start of the record

- D Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm
- **Tnew** Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille ...

#### Details

Case 20 describes an ideal temperature sinusoid without distortion by either changes in growth rate or changes in  $\delta^{18}O_w$  but with an even smaller temperature amplitude.

Generated using the code in "Generate\_Case20.r" in dataraw

## Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

#### Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 21 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case21

## Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

**D47** clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm
- Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm

Tnew Age, in years relative to the start of the record

- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

## Details

Case 21 describes an ideal temperature sinusoid without distortion by either changes in growth rate or changes in  $\delta^{18}O_w$  but with an the smallest temperature amplitude.

Generated using the code in "Generate\_Case21.r" in dataraw

#### Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

Case22

Virtual dataset Case 22

## Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 22 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case22

## Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm
- Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

## Details

Case 22 describes an natural environment with temperature and  $\delta^{18}O_w$  records from a tidal inlet (Texel harbor). data from inst/extdata/Texel\_data.csv.

Generated using the code in "Generate\_Case22.r" in dataraw

## Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

Case23

Virtual dataset Case 23

## Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 23 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case23

## Format

A data frame with 1200 rows and 30 variables:

SR\_ 0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

Tnew Age, in years relative to the start of the record

D Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm

Tnew Age, in years relative to the start of the record

- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille ...

## Details

Case 23 describes an natural environment with temperature and  $\delta^{18}O_w$  records from a tropical sea (Great Barrier Reef). data from inst/extdata/GBR\_data.csv.

Generated using the code in "Generate\_Case23.r" in dataraw

## Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

#### Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 24 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case24

#### Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

**D47** clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm
- **Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

#### Details

Case 24 describes an natural environment with temperature and  $\delta^{18}O_w$  records from an evaporation-dominated sea (Red Sea) data from inst/extdata/Red\_sea\_data.csv.

Generated using the code in "Generate\_Case24.r" in dataraw

#### Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

Case25

Virtual dataset Case 25

## Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 25 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case25

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

# Details

Case 25 describes an natural environment with temperature and  $\delta^{18}O_w$  records from a high-latitude marine site (Iceland). data from inst/extdata/Iceland\_data.csv.

Generated using the code in "Generate\_Case25.r" in dataraw

# Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

Case26

Virtual dataset Case 26

# Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 26 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

## Usage

Case26

# Format

A data frame with 1200 rows and 30 variables:

SR\_ 0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

Tnew Age, in years relative to the start of the record

D Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm

Tnew Age, in years relative to the start of the record

- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm
- **Tnew** Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille ...

# Details

Case 26 describes an ideal temperature sinusoid without distortion by either changes in growth rate or changes in  $\delta^{18}O_w$  but with a shorter (6 yr) record length.

Generated using the code in "Generate\_Case26.r" in dataraw

# Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

#### Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 27 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case27

# Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

**D47** clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

**D47** clumped isotope value, in permille

- SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm
- Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm

Tnew Age, in years relative to the start of the record

- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

# Details

Case 27 describes an ideal temperature sinusoid without distortion by either changes in growth rate or changes in  $\delta^{18}O_w$  but with a shorter (3 yr) record length.

Generated using the code in "Generate\_Case27.r" in dataraw

## Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

Case28

Virtual dataset Case 28

# Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 28 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case28

# Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm
- Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

# Details

Case 28 describes an ideal temperature sinusoid without distortion by either changes in growth rate or changes in  $\delta^{18}O_w$  but with a shorter (1 yr) record length.

Generated using the code in "Generate\_Case28.r" in dataraw

# Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

Case29

Virtual dataset Case 29

# Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 29 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

## Usage

Case29

# Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

D Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

**D47** clumped isotope value, in permille

SR\_ 0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm

Tnew Age, in years relative to the start of the record

- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm
- Tnew Age, in years relative to the start of the record
- D Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- **Tnew** Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille ...

## Details

Case 29 describes an ideal temperature sinusoid without distortion by changes in growth rate, but with seasonal variability in  $\delta^{18}O_w$  with a minimum in spring season and a tiny (1 days SD) error on age model

Generated using the code in "Generate\_Case29.r" in dataraw

## Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

#### Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 3 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case3

# Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

**D47** clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm
- **Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

#### Details

Case 3 describes an ideal temperature sinusoid without distortion by changes in  $\delta^{18}O_w$ , but with a growth stop in the warm season.

Generated using the code in "Generate\_Case3.r" in dataraw

## Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

Case30

Virtual dataset Case 30

# Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 30 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case30

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

# Details

Case 30 describes an ideal temperature sinusoid without distortion by changes in growth rate, but with seasonal variability in  $\delta^{18}O_w$  with a minimum in spring season and a small (5 days SD) error on age model (roughly +/– one week)

Generated using the code in "Generate\_Case30.r" in dataraw

## Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

Case31

Virtual dataset Case 31

## Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 31 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

## Usage

Case31

# Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm

- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille ...

# Details

Case 31 describes an ideal temperature sinusoid without distortion by changes in growth rate, but with seasonal variability in  $\delta^{18}O_w$  with a minimum in spring season and a larger (15 days SD) error on age model (roughly +/– one month)

Generated using the code in "Generate\_Case31.r" in dataraw

## Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

#### Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 32 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case32

## Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

**D47** clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm
- **Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm

Tnew Age, in years relative to the start of the record

- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

# Details

Case 32 describes an ideal temperature sinusoid without distortion by changes in growth rate, but with seasonal variability in  $\delta^{18}O_w$  with a minimum in spring season and a large (45 days SD) error on age model (roughly +/– three months)

Generated using the code in "Generate\_Case32.r" in dataraw

## Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

Case33

Virtual dataset Case 33

# Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 33 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

## Usage

Case33

# Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm
- Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

# Details

Case 33 describes an ideal temperature sinusoid without distortion by changes in growth rate, but with seasonal variability in  $\delta^{18}O_w$  with a minimum in spring season and a enormous (90 days SD) error on age model (roughly +/– half year)

Generated using the code in "Generate\_Case33.r" in dataraw

## Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

Case4

Virtual dataset Case 4

## Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 4 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

## Usage

Case4

# Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm

- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm
- Tnew Age, in years relative to the start of the record
- D Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille ...

# Details

Case 4 describes an ideal temperature sinusoid without distortion by changes in  $\delta^{18}O_w$ , but with a linearly decreasing growth rate.

Generated using the code in "Generate\_Case4.r" in dataraw

#### Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

#### Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 5 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case5

## Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

**D47** clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm
- **Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

#### Details

Case 5 describes an ideal temperature sinusoid without distortion by changes in  $\delta^{18}O_w$ , but with seasonal variability in growth rate which is in phase with the temperature seasonality.

Generated using the code in "Generate\_Case5.r" in dataraw

## Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

Case6

Virtual dataset Case 6

## Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 6 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case6

# Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

# Details

Case 6 describes an ideal temperature sinusoid without distortion by changes in  $\delta^{18}O_w$ , but with seasonal variability in growth rate which is in phase with maxima in the spring season.

Generated using the code in "Generate\_Case6.r" in dataraw

# Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

Case7

Virtual dataset Case 7

# Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 7 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

## Usage

Case7

# Format

A data frame with 1200 rows and 30 variables:

SR\_ 0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

Tnew Age, in years relative to the start of the record

D Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm

Tnew Age, in years relative to the start of the record

- D Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm
- **Tnew** Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille
- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record
- d18Oc stable oxygen isotope value, in permille VPDB
- D47 clumped isotope value, in permille ...

# Details

Case 7 describes an ideal temperature sinusoid without distortion by changes in growth rate, but with seasonal variability in  $\delta^{18}O_w$  in phase with temperature seasonality.

Generated using the code in "Generate\_Case7.r" in dataraw

## Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

#### Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 8 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case8

#### Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

**Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

**D47** clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm
- **Tnew** Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

**d18Oc** stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm
- Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

- D47 clumped isotope value, in permille
- SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

#### Details

Case 8 describes an ideal temperature sinusoid without distortion by changes in growth rate, but with seasonal variability in  $\delta^{18}O_w$  in antiphase with temperature seasonality.

Generated using the code in "Generate\_Case8.r" in dataraw

## Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

Case9

Virtual dataset Case 9

# Description

A dataset containing ages (Tnew), depth values (D), stable oxygen isotope values ( $\delta^{18}O$ ) and clumped isotope values  $\Delta_{47}$  of a simulated carbonate record based on environmental parameters following Case 9 and employing a sampling resolution of 0.1 mm, 0.2 mm, 0.45 mm, 0.75 mm, 1.55 mm and 3.25 mm.

#### Usage

Case9

# Format

A data frame with 1200 rows and 30 variables:

SR\_0.1 Empty column denoting the start of the record sampled at a sampling resolution of 0.1 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_0.2 Empty column denoting the start of the record sampled at a sampling resolution of 0.2 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.45 Empty column denoting the start of the record sampled at a sampling resolution of 0.45 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 0.75 Empty column denoting the start of the record sampled at a sampling resolution of 0.75 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

SR\_ 1.55 Empty column denoting the start of the record sampled at a sampling resolution of 1.55 mm

Tnew Age, in years relative to the start of the record

**D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille

- SR\_ 3.25 Empty column denoting the start of the record sampled at a sampling resolution of 3.25 mm
- Tnew Age, in years relative to the start of the record
- **D** Depth, in mm along the virtual record

d18Oc stable oxygen isotope value, in permille VPDB

D47 clumped isotope value, in permille ...

Case 9 describes an ideal temperature sinusoid without distortion by changes in growth rate, but with seasonal variability in  $\delta^{18}O_w$  with a minimum in spring season.

Generated using the code in "Generate\_Case9.r" in dataraw

## Source

See code to generate data in dataraw Details on how these example cases are defined is provided in:

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

optimization\_seasonality

Function for sample size optimization based clumped isotope seasonality reconstruction.

# Description

Combines records of stable oxygen isotope ratios ( $\delta^{18}O_c$ ) and clumped isotope ratios ( $\Delta_{47}$ ) through subannually resolved carbonate archives (e.g. mollusk shells or corals) to reconstruct monthly variability in temperature and salinity (through the  $\delta^{18}O$  composition of the precipitation fluid), using the sample size optimization method detailed in de Winter et al., 2020 (Climate of the Past).

#### Usage

```
optimization_seasonality(
    d180c,
    D47,
    ages,
    SD_d180c = 0.1,
    SD_D47 = 0.04,
    N = 1000,
    p = 0.05,
    d180_fun = "KimONeil97",
    D47_fun = "Bernasconi18",
    export = FALSE,
    export_raw = FALSE
)
```

## Arguments

d180c	Vector containing subannually resolved $\delta^{18}O_c$ data
D47	Vector containing subannually resolved $\Delta_{47}$ data
ages	Vector containing ages for of all samples in years relative to the shell chronology

SD_d180c	Error on the $\delta^{18}O_c$ measurements. Either a single value (constant uncertainty) or a vector of length equal to the period in SST data (365 days by default) contain- ing information about the error of each datapoint (1 standard deviation; default = 0.1 permille).
SD_D47	Error on the $\Delta_{47}$ measurements. Either a single value (constant uncertainty) or a vector of length equal to the period in SST data (365 days by default) containing information about the error of each datapoint (1 standard deviation; default = 0.04 permille).
Ν	Number of datapoints for Monte Carlo simulation (defaults to 1000)
р	Threshold value for the p value of separating summer from winter reconstruc- tions. Defaults to 0.05 (95% confidence level)
d180_fun	String containing the name of the transfer function used to convert temperature and $\delta^{18}O_w$ to $\delta^{18}O_c$ data (for example: "KimONeil97" or "GrossmanKu86"). Defaults to Kim and O'Neil (1997).
D47_fun	String containing the name of the transfer function used to convert temperature to $\Delta_{47}$ data (for example: "Bernasconi18" or "Jautzy20"). Defaults to Bernasconi et al., 2018).
export	Export table summary of result (CSV format)? TRUE/FALSE
export_raw	Export tables containing all raw model results before being merged into tidy tables? TRUE/FALSE

#### Value

A data frame containing monthly reconstructions of  $\Delta_{47}$ , temperature,  $\delta^{18}O$  of the precipitation fluid and  $\delta^{18}O_c$ .

## References

package dependencies: TTR Grossman, E.L., Ku, T., Oxygen and carbon isotope fractionation in biogenic aragonite: temperature effects, *Chemical Geology* **1986**, *59.1*, 59–74. https://doi.org/bvpzws

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de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

## Examples

```
# find attached dummy data
Case1 <- seasonalclumped::Case1</pre>
d180c <- Case1[, 29]
d180c <- d180c[-which(is.na(d180c))]</pre>
D47 <- Case1[, 30]
D47 <- D47[-which(is.na(D47))]
ages <- Case1[, 27]
ages <- ages[-which(is.na(ages))]</pre>
# Run function
monthly <- optimization_seasonality(d180c = d180c,</pre>
D47 = D47,
ages = ages,
SD_d180c = 0.1,
SD_D47 = 0.04,
N = 100, # Use small amount of samples for quick testing (recommended N = 1000)
p = 0.05,
d180_fun = "KimONeil97",
D47_fun = "Bernasconi18",
export = FALSE,
export_raw = FALSE)
```

oxygen\_isotope\_seasonality Function for oxygen isotope based seasonality reconstructions.

# Description

Uses records of stable oxygen isotope ratios ( $\delta^{18}O_c$ ) through subannually resolved carbonate archives (e.g. mollusk shells or corals) to reconstruct monthly variability in temperature and salinity (assuming user provided variability in  $\delta^{18}O$  composition of the precipitation fluid).

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# Usage

```
oxygen_isotope_seasonality(
    d180c,
    ages,
    SD_d180c = 0.1,
    d180w = 0,
    d180_fun = "KimONeil97",
    export = FALSE
)
```

# Arguments

d180c	Vector containing subannually resolved $\delta^{18}O_c$ data
ages	Vector containing ages for of all samples in years relative to the shell chronology
SD_d180c	Error on the $\delta^{18}O_c$ measurements. Either a single value (constant uncertainty) or a vector of length equal to the period in SST data (365 days by default) containing information about the error of each datapoint (1 standard deviation; default = 0.1 permille).
d180w	Vector containing $\delta^{18}O$ values (in permille VSMOW) of the precipitation fluid used to calculate temperatures. If only a single value is provided, the $\delta^{18}O$ of the fluid is presumed constant at this value. Default = 0 permille VSMOW.
d180_fun	String containing the name of the transfer function used to convert temperature and $\delta^{18}O_w$ to $\delta^{18}O_c$ data (for example: "KimONeil97" or "GrossmanKu86"). Defaults to Kim and O'Neil (1997).
export	Export table summary of result (CSV format)? TRUE/FALSE

# Value

A data frame containing monthly reconstructions of temperature,  $\delta^{18}O$  of the precipitation fluid and  $\delta^{18}O_c$ .

# References

Grossman, E.L., Ku, T., Oxygen and carbon isotope fractionation in biogenic aragonite: temperature effects, *Chemical Geology* **1986**, *59.1*, 59–74. https://doi.org/bvpzws

Kim, S., O'Niel, J.R., Equilibrium and nonequilibrium oxygen isotope effects in synthetic carbonates, *Geochimica et Cosmochimica Acta* **1997**, *61.16*, 3461–3475. https://doi.org/c7bwbp

Dettman, D.L., Reische, A.K., Lohmann, K.C., Controls on the stable isotope composition of seasonal growth bands in aragonitic fresh-water bivalves (Unionidae), *Geochimica et Cosmochimica Acta* **1999**, *63.7–8*, 1049–1057. https://doi.org/cbb7zc

Brand, W.A., Coplen, T.B., Vogl, J., Rosner, M., Prohaska, T., Assessment of international reference materials for isotope–ratio analysis (IUPAC Technical Report), *Pure and Applied Chemistry* **2014**, *86.3*, 425–467. https://doi.org/fpc2

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

# Examples

```
# find attached dummy data
Case1 <- seasonalclumped::Case1
d180c <- Case1[, 29]
d180c <- d180c[-which(is.na(d180c))]
ages <- Case1[, 27]
ages <- ages[-which(is.na(ages))]
# Run function
monthly <- oxygen_isotope_seasonality(d180c,
ages,
0.1,
0,
"KimONei197",
FALSE)
```

smoothing\_seasonality Function for sample size optimization based clumped isotope seasonality reconstruction.

# Description

Combines records of stable oxygen isotope ratios ( $\delta^{18}O_w$ ) and clumped isotope ratios (D47) through subannually resolved carbonate archives (e.g. mollusk shells or corals) to reconstruct monthly variability in temperature and salinity (through the  $\delta^{18}O$  composition of the precipitation fluid), using the moving average method detailed in de Winter et al., 2020 (Climate of the Past).

# Usage

```
smoothing_seasonality(
    d180c,
    D47,
    ages,
    SD_d180c = 0.1,
    SD_D47 = 0.04,
    window = "optimize",
    N = 1000,
    p = 0.05,
    d180_fun = "KimONeil97",
    D47_fun = "Bernasconi18",
    export = FALSE,
    export_raw = FALSE
)
```

# Arguments

d180c	Vector containing subannually resolved $\delta^{18}O_w$ data
D47	Vector containing subannually resolved D47 data

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ages	Vector containing ages for of all samples in years relative to the shell chronology
SD_d180c	Error on the $\delta^{18}O_w$ measurements. Either a single value (constant uncertainty) or a vector of length equal to the period in SST data (365 days by default) containing information about the error of each datapoint (1 standard deviation; default = 0.1 permille).
SD_D47	Error on the D47 measurements. Either a single value (constant uncertainty) or a vector of length equal to the period in SST data (365 days by default) containing information about the error of each datapoint (1 standard deviation; default = $0.04$ permille).
window	Either supply the size of the window used for moving average calculation (inte- ger with values between 2 and the length of the record), or enter the term "opti- mize" to let the function find the optimum window size for the record through a Monte Carlo approach.
Ν	Number of datapoints for Monte Carlo simulation (defaults to 1000)
р	Threshold value for the p value of separating summer from winter reconstructions. Defaults to $0.05~(95\%$ confidence level)
d180_fun	String containing the name of the transfer function used to convert temperature and $\delta^{18}O_w$ to $\delta^{18}O_w$ data (for example: "KimONeil97" or "GrossmanKu86"). Defaults to Kim and O'Neil (1997).
D47_fun	String containing the name of the transfer function used to convert tempera- ture to D47 data (for example: "Bernasconi18" or "Jautzy20"). Defaults to Bernasconi et al., 2018).
export	Export table summary of result (CSV format)? TRUE/FALSE
export_raw	Export tables containing all raw model results before being merged into tidy tables? TRUE/FALSE

# Value

A data frame containing monthly reconstructions of D47, temperature,  $\delta^{18}O$  of the precipitation fluid and  $\delta^{18}O_w$ .

#### References

package dependencies: TTR Grossman, E.L., Ku, T., Oxygen and carbon isotope fractionation in biogenic aragonite: temperature effects, *Chemical Geology* **1986**, *59.1*, 59–74. https://doi.org/bvpzws

Kim, S., O'Niel, J.R., Equilibrium and nonequilibrium oxygen isotope effects in synthetic carbonates, *Geochimica et Cosmochimica Acta* **1997**, *61.16*, 3461–3475. https://doi.org/c7bwbp

Dettman, D.L., Reische, A.K., Lohmann, K.C., Controls on the stable isotope composition of seasonal growth bands in aragonitic fresh-water bivalves (Unionidae), *Geochimica et Cosmochimica Acta* **1999**, *63.7–8*, 1049–1057. https://doi.org/cbb7zc

Brand, W.A., Coplen, T.B., Vogl, J., Rosner, M., Prohaska, T., Assessment of international reference materials for isotope–ratio analysis (IUPAC Technical Report), *Pure and Applied Chemistry* **2014**, *86.3*, 425–467. https://doi.org/fpc2

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Jautzy, J. J., Savard, M. M., Dhillon, R. S., Bernasconi, S. M. and Smirnoff, A., Clumped isotope temperature calibration for calcite: Bridging theory and experimentation, *Geochemical Perspectives Letters* **2020**, 14, 36–41. https://doi.org/fpc3

de Winter, N. J., Agterhuis, T., Ziegler, M., Optimizing sampling strategies in high-resolution paleoclimate records, *Climate of the Past Discussions* **2020**, 1–52. https://doi.org/fpc4

# Examples

```
# find attached dummy data
Case1 <- seasonalclumped::Case1</pre>
d180c <- Case1[, 29]
d180c <- d180c[-which(is.na(d180c))]</pre>
D47 <- Case1[, 30]
D47 <- D47[-which(is.na(D47))]
ages <- Case1[, 27]
ages <- ages[-which(is.na(ages))]</pre>
# Run function
monthly <- smoothing_seasonality(d180c,</pre>
D47,
ages,
0.1,
0.04,
"optimize",
100, # Use small amount of samples for quick testing (recommended N = 1000)
0.05,
"KimONeil97",
"Bernasconi18"
FALSE,
FALSE)
```

subsample

# Description

Function used to linearly subsample data at new depth values

## Usage

```
subsample(data, old_depth, new_depth, AV = FALSE, plot = FALSE)
```

## Arguments

data	A vector of data to be interpolated
old_depth	A vector containing the depth values belonging to data
new_depth	A vector containing depth values at which the data should be interpolated.
AV	Should the subsampling take into account the mean value within the sample in- terval? TRUE/FALSE If FALSE, the interpolated value corresponding to the exact position is used instead of the mean of the interval
plot	Should the result be plotted? TRUE/FALSE

# Value

A vector listing the values interpolated from data at the positions of new\_depth

## Examples

```
# Create test data (= ideal case)
# Set boundary conditions
Td <- seq(1, 12 * 365, 1) # Create timeline of 12 years in days
Ty <- Td / 365 # Convert to years
MAT <- 20 # Set mean annual temperature
Amp <- 10 # Set seasonal amplitude
Sext <- 2 * Amp # Calculate extent of seasonal variability</pre>
TSD <- 1.5 # Set the degree of random non–seasonal noise on the SST curve
# ("weather")
SST <- rnorm(length(Ty), MAT + Amp * sin(2 * pi * Ty), TSD) # Create virtual</pre>
# daily SST data
GR <- rep(10 / 365, length(Ty)) # Set growth rate to 10 mm/yr and create daily
# GR vector
SR <- 0.75 # Set sampling resolution to 0.75 mm
# Create vector for all samples along entire shell length by applying constant
# sampling resolution
D \le seq(SR, sum(GR), SR)
D_cum <- cumsum(GR) # Create cumulative depth vector for all values</pre>
new_data <- subsample(SST, D_cum, D, AV = TRUE, plot = FALSE) # Interpolate</pre>
# SST values at the positions of D while calculating sample averages
```

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