# Package: rsofun (via r-universe)

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Title The P-Model and BiomeE Modelling Framework

Version 5.0.0.9000

Description Implements the Simulating Optimal FUNctioning framework for site-scale simulations of ecosystem processes, including model calibration. It contains 'Fortran 90' modules for the P-model (Stocker et al. (2020) <doi:10.5194/gmd-13-1545-2020>), SPLASH (Davis et al. (2017) <doi:10.5194/gmd-10-689-2017>) and BiomeE (Weng et al. (2015) <doi:10.5194/bg-12-2655-2015>).

URL https://github.com/geco-bern/rsofun

BugReports https://github.com/geco-bern/rsofun/issues

License GPL-3

**Depends** R (>= 4.1.0)

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biomee\_gs\_leuning\_drivers

rsofun BiomeE driver data (Leuning photosynthesis model)

# Description

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Small dataset representing the driver to run the BiomeE-model at the CH-LAE site using the Leuning photosynthesis specification (and half-hourly time step) It can also be used together with leaf trait data from CH-LAE (biomee\_validation) to optimize model parameters.

## Usage

biomee\_gs\_leuning\_drivers

## Format

A tibble of driver data.

sitename Site name

params\_siml Simulation parameters as a data.frame, including the following data:

spinup Flag indicating whether this simulation does spin-up.

spinupyears Number of spin-up years.

recycle Number of first N years of forcing data.frame that are recycled for spin-up.

- **firstyeartrend** Year of first transient year (AD) (optional). Is only used to set years in output data frames. Defaults to 0 if not provided.
- **nyeartrend** Number of transient years (optional). Determines the length of simulation output after spin-up. Defaults to number of years contained in the forcing data. (If longer than forcing data, last year of forcing is repeated until the end (spin-down).)
- steps\_per\_day Time resolution of the forcing (day-1).
- do\_U\_shaped\_mortality Flag indicating whether U-shaped mortality is used.
- **update\_annualLAImax** Flag indicating whether updating LAImax according to mineral N in soil.
- **do\_closedN\_run** Flag indicating whether doing N closed runs to recover N balance enforcing 0.2 kg N m-2 in the inorganic N pool.
- code\_method\_photosynth String specifying the method of photosynthesis used in the model, either "pmodel" or "gs\_leuning".document()
- **code\_method\_mortality** String indicating the type of mortality in the model. One of the following: "dbh" is size-dependent mortality, "const\_selfthin" is constant self thinning (in development), "cstarvation" is carbon starvation, and "growthrate" is growth rate dependent mortality.
- site\_info Site meta info in a data.frame. This data structure can be freely used for documenting the dataset, but must include at least the following data:

**lon** Longitude of the site location in degrees east.

lat Latitude of the site location in degrees north.

elv Elevation of the site location, in meters above sea level.

forcing Forcing data.frame used as input

**ppfd** Photosynthetic photon flux density (mol s-1 m-2)

tair Air temperature (deg C)

- vpd Vapor pressure deficit (Pa)
- **rain** Precipitation (kgH2O m-2 s-1 == mm s-1)

wind Wind velocity (m s-1)

**pair** Atmospheric pressure (pa)

**co2** CO2 atmospheric concentration (ppm)

- **params\_tile** Tile-level model parameters, into a single row data.frame, including the following data:
  - **soiltype** Integer indicating the type of soil: Sand = 1, LoamySand = 2, SandyLoam = 3, SiltLoam = 4, FrittedClay = 5, Loam = 6, Clay = 7.
  - **FLDCAP** Field capacity (vol/vol). Water remaining in a soil after it has been thoroughly saturated and allowed to drain freely.
  - **WILTPT** Wilting point (vol/vol). Water content of a soil at which plants wilt and fail to recover.
  - **K1** Fast soil C decomposition rate (year $^{-1}$ ).
  - **K2** Slow soil C decomposition rate (year $^{-1}$ ).
  - **K\_nitrogen** Mineral Nitrogen turnover rate (year $^{-1}$ ).

MLmixRatio Ratio of C and N returned to litters from microbes.

etaN N loss rate through runoff (organic and mineral) (year $^{-1}$ ). **LMAmin** Minimum LMA, leaf mass per unit area, kg C m $^{-2}$ . fsc\_fine Fraction of fast turnover carbon in fine biomass. fsc wood Fraction of fast turnover carbon in wood biomass. **GR\_factor** Growth respiration factor. **l fract** Fraction of the carbon retained after leaf drop. retransN Retranslocation coefficient of nitrogen. **f\_initialBSW** Coefficient for setting up initial sapwood. **f** N add Re-fill of N for sapwood. tf\_base Calibratable scalar for respiration, used to increase LUE levels. par mort Canopy mortality parameter. par\_mort\_under Parameter for understory mortality. params\_species A data.frame containing species-specific model parameters, with one species per row, including the following data: lifeform Integer set to 0 for grasses and 1 for trees. **phenotype** Integer set to 0 for deciduous and 1 for evergreen. pt Integer indicating the type of plant according to photosynthesis: 0 for C3; 1 for C4 **alpha FR** Fine root turnover rate (year $^{-1}$ ). **rho\_FR** Material density of fine roots (kg C  $m^{-3}$ ). root\_r Radius of the fine roots, in m. root zeta e-folding parameter of root vertical distribution, in m. **Kw root** Fine root water conductivity (mol  $m^{-2} s^{-1} MPa^{-1}$ ). leaf size Characteristic leaf size. **Vmax** Max RuBisCo rate, in mol  $m^{-2} s^{-1}$ . **Vannual** Annual productivity per unit area at full sun (kg C m<sup>-2</sup> year<sup>-2</sup>). wet\_leaf\_dreg Wet leaf photosynthesis down-regulation. m cond Factor of stomatal conductance. alpha\_phot Photosynthesis efficiency. **gamma** L Leaf respiration coefficient, in year $^{-1}$ . gamma\_LN Leaf respiration coefficient per unit N. **gamma SW** Sapwood respiration rate, in kg C m $^{-2}$  year $^{-1}$ . **gamma\_FR** Fine root respiration rate, kg C kg  $C^{-1}$  year<sup>-1</sup>. tc\_crit Critical temperature triggerng offset of phenology, in Kelvin. tc\_crit\_on Critical temperature triggerng onset of phenology, in Kelvin. gdd\_crit Critical value of GDD5 for turning ON growth season. betaON Critical soil moisture for phenology onset. betaOFF Critical soil moisture for phenology offset. seedlingsize Initial size of seedlings, in kg C per individual. **LNbase** Basal leaf N per unit area, in kg N  $m^{-2}$ . lAImax Maximum crown LAI (leaf area index). **Nfixrate0** Reference N fixation rate (kg N kg  $C^{-1}$  root). **NfixCost0** Carbon cost of N fixation (kg C kg  $N^{-1}$ ).

phiCSA Ratio of sapwood area to leaf area. **mortrate d c** Canopy tree mortality rate (year $^{-1}$ ). **mortrate d u** Understory tree mortality rate (year $^{-1}$ ). **maturalage** Age at which trees can reproduce (years). v\_seed Fraction of G\_SF to G\_F. fNSmax Multiplier for NSNmax as sum of potential bl and br. **LMA** Leaf mass per unit area (kg C  $m^{-2}$ ). **rho\_wood** Wood density (kg C  $m^{-3}$ ). **alphaBM** Coefficient for allometry (biomass = alphaBM \* DBH \*\* thetaBM). thetaBM Coefficient for allometry (biomass = alphaBM \* DBH \*\* thetaBM). **kphio** Quantum yield efficiency  $\varphi_0$ , in mol mol<sup>-1</sup>. phiRL Ratio of fine root to leaf area. LAI light Maximum LAI limited by light. init\_cohort A data.frame of initial cohort specifications, including the following data: init\_cohort\_species Index of a species described in param\_species. **init\_cohort\_nindivs** Initial individual density, in individuals per m<sup>2</sup>. init cohort bl Initial biomass of leaf, in kg C per individual. init cohort br Initial biomass of fine root, in kg C per individual. init\_cohort\_bsw Initial biomass of sapwood, in kg C per individual. init\_cohort\_bHW Initial biomass of heartwood, in kg C per individual. init\_cohort\_seedC Initial biomass of seed, in kg C per individual. init\_cohort\_nsc Initial non-structural biomass, in kg C per individual. init soil A data.frame of initial soil pools, including the following data: **init\_fast\_soil\_C** Initial fast soil carbon, in kg C m<sup>-2</sup>. init slow soil C Initial slow soil carbon, in kg C m $^{-2}$ . **init\_Nmineral** Mineral nitrogen pool, in kg N  $m^{-2}$ . **N** input Annual nitrogen input to soil N pool, in kg N m<sup>-2</sup> year<sup>-1</sup>.

biomee\_gs\_leuning\_output

rsofun BiomeE (gs\_leuning) output data

#### Description

Example output dataset from a BiomeE-model run (gs\_leuning) See run\_biomee\_f\_bysite for a detailed description of the outputs.

#### Usage

biomee\_gs\_leuning\_output

#### Format

An object of class tbl\_df (inherits from tbl, data.frame) with 1 rows and 2 columns.

```
biomee_p_model_drivers
```

rsofun BiomeE driver data (P-model photosynthesis model)

## Description

Small dataset representing the driver to run the BiomeE-model at the CH-LAE site using the P-model photosynthesis specification (and daily time step). It can also be used together with leaf trait data from CH-LAE (biomee\_validation) to optimize model parameters.

## Usage

```
biomee_p_model_drivers
```

## Format

See biomee\_gs\_leuning\_drivers

biomee\_p\_model\_output rsofun BiomeE (P-model) output data

# Description

Example output dataset from a BiomeE-model run (p-model) See run\_biomee\_f\_bysite for a detailed description of the outputs.

## Usage

```
biomee_p_model_output
```

## Format

An object of class tbl\_df (inherits from tbl, data.frame) with 1 rows and 2 columns.

biomee\_validation rsofun BiomeE targets validation data

## Description

Small example dataset of target observations (leaf trait data) at the CH-LAE site to optimize model parameters with the function calib\_sofun

## Usage

biomee\_validation

#### Format

A tibble of validation data:

sitename site name

data validation data

## Source

Lukas Hörtnagl, Werner Eugster, Nina Buchmann, Eugenie Paul-Limoges, Sophia Etzold, Matthias Haeni, Peter Pluess, Thomas Baur (2004-2014) FLUXNET2015 CH-Lae Laegern, Dataset. https://doi.org/10.18140/FLX/144

calib\_sofun Calibrates SOFUN model parameters

## Description

This is the main function that handles the calibration of SOFUN model parameters.

## Usage

```
calib_sofun(drivers, obs, settings, optim_out = TRUE, ...)
```

#### Arguments

drivers	A data frame with driver data. See p_model_drivers for a description of the data structure.
obs	A data frame containing observational data used for model calibration. See p_model_validation for a description of the data structure.
settings	A list containing model calibration settings. See the 'P-model usage' vignette for more information and examples.
	${\tt method} \ \ A \ string \ indicating \ the \ optimization \ method, \ either \ {\tt GenSA' \ or \ BayesianTools'}.$

	par A list of model parameters. For each parameter, an initial value and lower and upper bounds should be provided. The calibratable parameters include model parameters 'kphio', 'kphio_par_a', 'kphio_par_b', 'soilm_thetastar', 'soilm_betao', 'beta_costunitratio', 'rd_to_vcmax', 'tau_acclim', 'kc_jmax' and 'rootzone_whc', and (if doing Bayesian calibration) error parameters for each target variable, named for example 'err_gpp'. This list must match the input parameters of the calibration metric and the parameters should be given in the order above.
	metric A cost function. See the 'Cost functions for parameter calibration' vi- gnette for examples.
	<pre>control A list of arguments passed on to the optimization function. If method = 'GenSA', see GenSA. If method = 'BayesianTools' the list should in- clude at least settings and sampler, see BayesianTools::runMCMC.</pre>
optim_out	A logical indicating whether the function returns the raw output of the optimiza- tion functions (defaults to TRUE).
	Optional arguments passed on to the cost function specified as settings\$metric.

## Value

•

A named list containing the calibrated parameter vector 'par' and the output object from the optimization 'mod'. For more details on this output and how to evaluate it, see runMCMC (also this post) and GenSA.

## Examples

```
# Fix model parameters that won't be calibrated
params_fix <- list(
 soilm_thetastar = 0.6*240,
                 = 0.01,
 soilm_betao
 beta_unitcostratio = 146,
 rd_to_vcmax = 0.014,
 tau_acclim
                   = 30,
 kc_jmax
                  = 0.41
)
# Define calibration settings
settings <- list(</pre>
 method = "BayesianTools",
 par = list(
   kphio = list(lower=0.04, upper=0.09, init=0.05),
   err_gpp = list(lower = 0.01, upper = 4, init = 2)
 ),
 metric = rsofun::cost_likelihood_pmodel,
 control = list(
   sampler = "DEzs",
   settings = list(
     nrChains = 1,
```

cost\_likelihood\_biomee

Log-likelihood cost function for BiomeE with different targets

## Description

Cost function for parameter calibration, which computes the log-likelihood for the biomee model fitting several target variables for a given set of parameters.

#### Usage

cost\_likelihood\_biomee(par, obs, drivers, targets)

## Arguments

par	A vector containing parameter values for 'phiRL', 'LAI_light', 'tf_base', 'par_mort' in that order, and for the error terms corresponding to the target variables, e.g. 'err_GPP' if GPP is a target. Make sure that the order of the error terms in par coincides with the order provided in the targets argument.
obs	A nested data frame of observations, following the structure of biomee_validation, for example.
drivers	A nested data frame of driver data, for example biomee_gs_leuning_drivers.
targets	A character vector indicating the target variables for which the optimization will be done. This should be a subset of c("GPP", "LAI", "Density", "Biomass").

## Details

The cost function performs a BiomeE model run for the value of par given as argument. The likelihood is calculated assuming that the predicted targets are independent, normally distributed and centered on the observations. The optimization should be run using BayesianTools, so the likelihood is maximized.

## Value

The log-likelihood of the simulated targets by the biomee model versus the observed targets.

## Examples

cost\_likelihood\_pmodel

*Cost function computing a log-likelihood for calibration of P-model parameters* 

#### Description

The cost function performs a P-model run for the input drivers and model parameter values, and computes the outcome's normal log-likelihood centered at the input observed values and with standard deviation given as an input parameter (calibratable).

## Usage

```
cost_likelihood_pmodel(
   par,
   obs,
   drivers,
   targets,
   par_fixed = NULL,
   parallel = FALSE,
   ncores = 2
)
```

## Arguments

```
par
```

A vector of values for the parameters to be calibrated, including a subset of model parameters (described in runread\_pmodel\_f), in order, and error terms for each target variable (for example 'gpp\_err'), in the same order as the targets appear in targets.

obs	A nested data.frame of observations, with columns 'sitename' and 'data' (see p_model_validation or p_model_validation_vcmax25 to check their structure).
drivers	A nested data.frame of driver data. See p_model_drivers for a description of the data structure.
targets	A character vector indicating the target variables for which the optimization will be done and the RMSE computed. This string must be a column name of the data data.frame belonging to the validation nested data.frame (for example 'gpp').
par_fixed	A named list of model parameter values to keep fixed during the calibration. These should complement the input par such that all model parameters are passed on to runread_pmodel_f.
parallel	A logical specifying whether simulations are to be parallelised (sending data from a certain number of sites to each core). Defaults to FALSE.
ncores	An integer specifying the number of cores used for parallel computing. Defaults to 2.

#### Details

To run the P-model, all model parameters must be given. The cost function uses arguments par and par\_fixed such that, in the calibration routine, par can be updated by the optimizer and par\_fixed are kept unchanged throughout calibration.

If the validation data contains a "date" column (fluxes), the simulated target time series is compared to the observed values on those same dates (e.g. for GPP). Otherwise, there should only be one observed value per site (leaf traits), and the outputs (averaged over the growing season, weighted by predicted GPP) will be compared to this single value representative of the site (e.g. Vcmax25). As an exception, when the date of a trait measurement is available, it will be compared to the trait value predicted on that date.

## Value

The log-likelihood of the observed target values, assuming that they are independent, normally distributed and centered on the predictions made by the P-model run with standard deviation given as input (via 'par' because the error terms are estimated through the calibration with 'BayesianTools', as shown in the "Parameter calibration and cost functions" vignette).

## Examples

```
par_fixed = list(
soilm_thetastar = 0.6 * 240, # old setup with soil moisture stress
soilm_betao = 0.0,
beta_unitcostratio = 146.0,
rd_to_vcmax = 0.014, # from Atkin et al. 2015 for C3 herbaceous
tau_acclim = 30.0,
kc_jmax = 0.41
)
```

cost\_rmse\_biomee RMSE cost function for BiomeE

#### Description

Cost function for parameter calibration, which computes the root mean squared error (RMSE) between BiomeE simulations (using the input set of parameters) and observed target variables. Cost function for parameter calibration, which computes the RMSE for the biomee model fitting target variables 'GPP', 'LAI', 'Density' and 'Biomass' for a given set of parameters.

#### Usage

cost\_rmse\_biomee(par, obs, drivers)

## Arguments

par	A vector containing parameter values for 'phiRL','LAI_light', 'tf_base', 'par_mort' in that order.
obs	A nested data frame of observations, following the structure of biomee_validation, for example.
drivers	A nested data frame of driver data, for example biomee_gs_leuning_drivers.

## Value

The root mean squared error (RMSE) between the observed and simulated values of 'GPP', 'LAI', 'Density' and 'Biomass' (all variables have the same weight). Relative errors (difference divided by observed values) are used instead of absolute errors. The cost function performs a BiomeE model run for parameter values par and model drivers drivers given as arguments, producing the simulated values used to compute the RMSE.

#### Examples

```
# Compute RMSE for a set of
# model parameter values
# and example data
cost_rmse_biomee(
  par = c(3.5, 3.5, 1, 1),
  obs = biomee_validation,
```

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```
drivers = biomee_gs_leuning_drivers
)
```

cost\_rmse\_pmodel Cost function computing RMSE for calibration of P-model parameters

# Description

The cost function performs a P-model run for the input drivers and parameter values, and compares the output to observations of various targets by computing the root mean squared error (RMSE).

## Usage

```
cost_rmse_pmodel(
  par,
  obs,
  drivers,
  targets,
  par_fixed = NULL,
  target_weights = NULL,
  parallel = FALSE,
  ncores = 2
)
```

## Arguments

par	A vector of values for the parameters to be calibrated (a subset of those described in runread_pmodel_f, in order).
obs	A nested data.frame of observations, with columns 'sitename' and 'data' (see p_model_validation or p_model_validation_vcmax25 to check their structure).
drivers	A nested data.frame of driver data. See p_model_drivers for a description of the data structure.
targets	A character vector indicating the target variables for which the optimization will be done and the RMSE computed. This string must be a column name of the data data.frame belonging to the validation nested data.frame (for example 'gpp').
par_fixed	A named list of model parameter values to keep fixed during the calibration. These should complement the input par such that all model parameters are passed on to runread_pmodel_f.
target_weights	A vector of weights to be used in the computation of the RMSE if using several targets. By default (target_weights = NULL) the RMSE is computed separately for each target and then averaged. The provided weights are used to compute a weighted average of RMSE across targets.

parallel	A logical specifying whether simulations are to be parallelised (sending data
	from a certain number of sites to each core). Defaults to FALSE.
ncores	An integer specifying the number of cores used for parallel computing. Defaults
	to 2.

#### Details

To run the P-model, all model parameters must be given. The cost function uses arguments par and par\_fixed such that, in the calibration routine, par can be updated by the optimizer and par\_fixed are kept unchanged throughout calibration.

If the validation data contains a "date" column (fluxes), the simulated target time series is compared to the observed values on those same dates (e.g. for GPP). Otherwise, there should only be one observed value per site (leaf traits), and the outputs (averaged over the growing season, weighted by predicted GPP) will be compared to this single value representative of the site (e.g. Vcmax25). As an exception, when the date of a trait measurement is available, it will be compared to the trait value predicted on that date.

## Value

The root mean squared error (RMSE) between observed values and P-model predictions. The RMSE is computed for each target separately and then aggregated (mean or weighted average).

#### Examples

```
# Compute RMSE for a set
# of model parameter values
# and example data
cost_rmse_pmodel(
par = c(0.05, -0.01, 0.5), # kphio related parameters
obs = p_model_validation,
drivers = p_model_drivers,
targets = c('gpp'),
par_fixed = list(
 soilm_thetastar
                    = 0.6 * 240, # old setup with soil moisture stress
 soilm_betao
                    = 0.0,
 beta_unitcostratio = 146.0,
                                  # from Atkin et al. 2015 for C3 herbaceous
 rd_to_vcmax
                   = 0.014,
                    = 30.0,
 tau_acclim
                    = 0.41
 kc_jmax
)
)
```

init\_dates\_dataframe Initialises a tibble with dates

## Description

Creates a tibble with rows for each date from 'yrstart' to 'yrend' in 'yyyy-mm-dd' format. Intervals of dates are specified by argument 'freq'. ddf <- init\_dates\_dataframe(2000, 2003, start-moy=1, startdoy=1, freq="days", endmoy=12, enddom=31, noleap=FALSE) p\_model\_drivers

## Usage

```
init_dates_dataframe(
  yrstart,
  yrend,
  startmoy = 1,
  startdoy = 1,
  freq = "days",
  endmoy = 12,
  enddom = 31,
  noleap = FALSE
```

```
)
```

## Arguments

yrstart	An integer defining the start year of dates covered by the dataframe.
yrend	An integer defining the end year of dates covered by the dataframe.
startmoy	An integer defining the start month-of-year of dates covered by the dataframe. Defaults to 1.
startdoy	An integer defining the start day-of-year of dates covered by the dataframe. De- faults to 1.
freq	A character string specifying the time steps of dates (in rows). Defaults to "days". Any of "days", "months", "years". If freq = "months" the $15^{th}$ day of the months is used as date, and if freq = "years" the $1^{st}$ of January of each year is returned.
endmoy	An integer defining the end month-of-year of dates covered by the dataframe. Defaults to 12.
enddom	An integer defining the end day-of-year of dates covered by the dataframe. De- faults to 31.
noleap	Whether leap years are ignored, that is, whether the $29^{th}$ of February is removed. Defaults to FALSE.

## Value

A tibble with dates.

p\_model\_drivers rsofun P-model driver data

## Description

Small dataset representing the driver to run the P-model at the FR-Pue site. It can also be used together with daily GPP flux time series data from CH-LAE (p\_model\_validation) to optimize model parameters. To optimize model parameters to leaf traits data use the datasets p\_model\_drivers\_vcmax25 and p\_model\_validation\_vcmax25.

#### Usage

p\_model\_drivers

## Format

A tibble of driver data:

sitename A character string containing the site name.

forcing A tibble of a time series of forcing climate data, including the following data:

date Date of the observation in YYYY-MM-DD format.

temp Daytime average air temperature in °C.

vpd Daytime average vapour pressure deficit in Pa.

**ppfd** Photosynthetic photon flux density (PPFD) in mol  $m^{-2} s^{-1}$ . If all values are NA, it indicates that PPFD should be calculated by the SPLASH model.

**netrad** Net radiation in W  $m^{-2}$ . This is currently ignored as a model forcing.

patm Atmospheric pressure in Pa.

**snow** Snow in water equivalents mm  $s^{-1}$ .

**rain** Rain as precipitation in liquid form in mm  $s^{-1}$ .

tmin Daily minimum air temperature in °C.

tmax Daily maximum air temperature in °C.

fapar Fraction of photosynthetic active radiation (fAPAR), taking values between 0 and 1.

**co2** Atmospheric CO<sub>2</sub> concentration.

- **ccov** Cloud coverage in %. This is only used when either PPFD or net radiation are not prescribed.
- params\_siml A tibble of simulation parameters, including the following data:

spinup A logical value indicating whether this simulation does spin-up.

spinupyears Number of spin-up years.

recycle Number of first N years of forcing data.frame that are recycled for spin-up.

outdt An integer indicating the output periodicity.

Itre A logical value, TRUE if evergreen tree.

**Itne** A logical value, TRUE if evergreen tree and N-fixing.

ltrd A logical value, TRUE if deciduous tree.

ltnd A logical value, TRUE if deciduous tree and N-fixing.

lgr3 A logical value, TRUE if grass with C3 photosynthetic pathway.

lgn3 A logical value, TRUE if grass with C3 photosynthetic pathway and N-fixing.

**lgr4** A logical value, TRUE if grass with C4 photosynthetic pathway.

**site\_info** A tibble containing site meta information. This data structure can be freely used for documenting the dataset, but must include at least the following data:

lon Longitude of the site location in degrees east.

**lat** Latitude of the site location in degrees north.

elv Elevation of the site location, in meters above sea level.

whc A numeric value for the rooting zone water holding capacity (in mm)

#### Source

Pastorello, G., Trotta, C., Canfora, E. et al. The FLUXNET2015 dataset and the ONEFlux processing pipeline for eddy covariance data. Sci Data 7, 225 (2020). https://doi.org/10.1038/s41597-020-0534-3

University of East Anglia Climatic Research Unit; Harris, I.C.; Jones, P.D.; Osborn, T. (2021): CRU TS4.05: Climatic Research Unit (CRU) Time-Series (TS) version 4.05 of high-resolution gridded data of month-by-month variation in climate (Jan. 1901- Dec. 2020). NERC EDS Centre for Environmental Data Analysis, date of citation. https://catalogue.ceda.ac.uk/uuid/c26a65020a5e4b80b20018f148556681

Weedon, G. P., G. Balsamo, N. Bellouin, S. Gomes, M. J. Best, and P. Viterbo(2014), The WFDEI meteorological forcing data set: WATCH Forcing Datamethodology applied to ERA-Interimreanalysis data, Water Resour. Res., 50, 7505–7514, doi:10.1002/2014WR015638.

Fick, S.E. and R.J. Hijmans, 2017. WorldClim 2: new 1km spatial resolution climate surfaces for global land areas. International Journal of Climatology 37 (12): 4302-4315.

p\_model\_drivers\_vcmax25

rsofun P-model driver data (for leaf traits)

#### Description

Small dataset representing the driver to run the P-model at four separate sites. It can also be used together with leaf traits data from these four sites (p\_model\_validation\_vcmax25) to optimize model parameters. To optimize model parameters to GPP flux data use the datasets p\_model\_drivers and p\_model\_validation.

#### Usage

p\_model\_drivers\_vcmax25

#### Format

See p\_model\_drivers

#### Source

Atkin, O. K., Bloomfield, K. J., Reich, P. B., Tjoelker, M. G., Asner, G. P., Bonal, D., et al. (2015). Global variability in leaf respiration in relation to climate, plant functional types and leaf traits. New Phytol. 206 (2), 614–636. doi:10.1111/nph.13253

University of East Anglia Climatic Research Unit; Harris, I.C.; Jones, P.D.; Osborn, T. (2021): CRU TS4.05: Climatic Research Unit (CRU) Time-Series (TS) version 4.05 of high-resolution gridded data of month-by-month variation in climate (Jan. 1901- Dec. 2020). NERC EDS Centre for Environmental Data Analysis, date of citation. https://catalogue.ceda.ac.uk/uuid/c26a65020a5e4b80b20018f148556681

Weedon, G. P., G. Balsamo, N. Bellouin, S. Gomes, M. J. Best, and P. Viterbo(2014), The WFDEI meteorological forcing data set: WATCH Forcing Datamethodology applied to ERA-Interimreanalysis data, Water Resour. Res., 50, 7505–7514, doi:10.1002/2014WR015638.

Fick, S.E. and R.J. Hijmans, 2017. WorldClim 2: new 1km spatial resolution climate surfaces for global land areas. International Journal of Climatology 37 (12): 4302-4315.

C.D. Keeling, R.B. Bacastow, A.E. Bainbridge, C.A. Ekdahl, P.R. Guenther, and L.S. Waterman, (1976), Atmospheric carbon dioxide variations at Mauna Loa Observatory, Hawaii, Tellus, vol. 28, 538-551

p\_model\_output rsofun P-model output data

### Description

Example output dataset from a p-model run using p\_model\_drivers See run\_pmodel\_f\_bysite for a detailed description of the outputs.

#### Usage

p\_model\_output

## Format

An object of class tbl\_df (inherits from tbl, data.frame) with 1 rows and 3 columns.

p\_model\_output\_vcmax25

rsofun P-model output data (using vcmax25 drivers)

## Description

Example output dataset from a p-model run using p\_model\_drivers\_vcmax25 See run\_pmodel\_f\_bysite for a detailed description of the outputs.

#### Usage

p\_model\_output\_vcmax25

#### Format

An object of class tbl\_df (inherits from tbl, data.frame) with 4 rows and 3 columns.

p\_model\_validation rsofun P-model GPP validation data

### Description

Small example dataset of target observations (daily GPP flux data) to optimize model parameters with the function calib\_sofun

#### Usage

p\_model\_validation

#### Format

A tibble of validation data:

sitename A character string containing the site name (e.g. 'FR-Pue').

data A tibble [2,920 x 3] with time series for the following variables:

date Date vector with format YYYY-MM-DD.

**gpp** The observed Gross Primary Productivity (GPP) for each time stamp (in gC m<sup>-2</sup> d<sup>-1</sup>). **gpp\_unc** The uncertainty of the GPP (in gC m<sup>-2</sup> d<sup>-1</sup>).

#### Source

Pastorello, G., Trotta, C., Canfora, E. et al. The FLUXNET2015 dataset and the ONEFlux processing pipeline for eddy covariance data. Sci Data 7, 225 (2020). https://doi.org/10.1038/s41597-020-0534-3

#### Examples

```
require(ggplot2); require(tidyr)
p_model_validation %>% tidyr::unnest(data)
```

p\_model\_validation\_vcmax25

rsofun P-model Vcmax25 validation data

#### Description

Small example dataset of target observations (leaf trait data) to optimize model parameters with the function calib\_sofun

#### Usage

p\_model\_validation\_vcmax25

## Format

A tibble of validation data:

- sitename A character string containing the site names (e.g. 'Reichetal\_Colorado').
- **data** A tibble [1 x 2] with observations for the following variables:
  - **vcmax25** The observed maximum rate of carboxylation (Vcmax), normalised to  $25^{\circ}$  C (in mol C m<sup>-2</sup> d<sup>-1</sup>), aggregated over different plant species in each site.
  - **vcmax25\_unc** The uncertainty of the Vcmax25 (in mol C m<sup>-2</sup> d<sup>-1</sup>), calculated as the standard deviation among Vcmax25 observations for several species per site or as the total standard deviation across sites for single-plant-species sites.

#### Source

Atkin, O. K., Bloomfield, K. J., Reich, P. B., Tjoelker, M. G., Asner, G. P., Bonal, D., et al. (2015). Global variability in leaf respiration in relation to climate, plant functional types and leaf traits. New Phytol. 206 (2), 614–636. doi:10.1111/nph.13253

## Examples

```
require(ggplot2); require(tidyr)
p_model_validation_vcmax25 %>% tidyr::unnest(data)
```

runread\_biomee\_f Run BiomeE

## Description

Runs BiomeE model for multiple sites.

#### Usage

```
runread_biomee_f(drivers, makecheck = TRUE, parallel = FALSE, ncores = 2)
```

## Arguments

drivers	A nested data frame with one row for each site and columns named according to the arguments of function run_biomee_f_bysite. Namely sitename, params_siml, site_info and forcing.
makecheck	A logical specifying whether checks are performed to verify forcings and model parameters. TRUE by default.
parallel	Flag specifying whether simulations are to be parallelised (sending data from a certain number of sites to each core). Defaults to FALSE.
ncores	An integer specifying the number of cores used for parallel computing. Defaults to 2.

## Value

A data frame (tibble) with one row for each site, site information stored in the nested column site\_info and model outputs stored in the nested column data. See run\_biomee\_f\_bysite for a detailed description of the outputs. Example outputs are provided as p\_model\_output and p\_model\_output\_vcmax25.

# Examples

# Example BiomeE model run

```
runread_biomee_f(
   drivers = biomee_gs_leuning_drivers
)
runread_biomee_f(
   drivers = biomee_p_model_drivers
)
```

runread\_pmodel\_f Run P-model

## Description

Runs P-model for multiple sites.

## Usage

```
runread_pmodel_f(drivers, par, makecheck = TRUE, parallel = FALSE, ncores = 1)
```

## Arguments

drivers	A nested data frame with one row for each site and columns named according to the arguments of function runread_pmodel_f. Namely sitename, params_siml, site_info and forcing.
par	A named list of free (calibratable) model parameters.
	<b>kphio</b> The quantum yield efficiency at optimal temperature $\varphi_0$ , in mol mol <sup>-1</sup> . When temperature dependence is used, it corresponds to the multiplicative parameter <i>c</i> (see Details).
	<b>kphio_par_a</b> The shape parameter <i>a</i> of the temperature-dependency of quantum yield efficiency (see Details). To disable the temperature dependence, set kphio_par_a = 0.
	<b>kphio_par_b</b> The optimal temperature parameter $b$ of the temperature dependent quantum yield efficiency (see Details), in ${}^{o}C$ .
	<b>soilm_thetastar</b> The threshold parameter $\theta^*$ in the soil moisture stress function (see Details), given in mm. To turn off the soil moisture stress, set soilm_thetastar = 0.

	<b>soilm_betao</b> The intercept parameter $\beta_0$ in the soil moisture stress function (see Details). This is the parameter calibrated in Stocker et al. 2020 GMD.
	<b>beta_unitcostratio</b> The unit cost of carboxylation, corresponding to $\beta = b/a'$ in Eq. 3 of Stocker et al. 2020 GMD.
	rd_to_vcmax Ratio of Rdark (dark respiration) to Vcmax25.
	tau_acclim Acclimation time scale of photosynthesis, in days.
	<b>kc_jmax</b> Parameter for Jmax cost ratio (corresponding to c* in Stocker et al. 2020 GMD).
makecheck	A logical specifying whether checks are performed to verify forcings and model parameters. TRUE by default.
parallel	A logical specifying whether simulations are to be parallelised (sending data from a certain number of sites to each core). Defaults to FALSE.
ncores	An integer specifying the number of cores used for parallel computing (by de-fault ncores = 2).

#### Details

Depending on the input model parameters, it's possible to run the different P-model setups presented in Stocker et al. 2020 GMD. The P-model version implemented in this package allows more flexibility than the one presented in the paper, with the following functions:

The temperature dependence of the quantum yield efficiency is given by:

$$\begin{split} \varphi_0(T) &= c(1+a(T-b)^2) \text{ if } 0 < c(1+a(T-b)^2) < 1, \\ \varphi_0(T) &= 0 \text{ if } c(1+a(T-b)^2) \le 0, \text{ and} \\ \varphi_0(T) &= 1 \text{ if } c(1+a(T-b)^2) \ge 1. \end{split}$$

The ORG setup can be reproduced by setting kphio\_par\_a = 0 and calibrating the kphio parameter only. The BRC setup (which calibrates  $c_L = \frac{a_L b_L}{4}$  in Eq. 18) is more difficult to reproduce, since the temperature-dependency has been reformulated and a custom cost function would be necessary for calibration. The new parameters are related to  $c_L$  as follows:

a = -0.0004919819

b = 32.35294

 $c = 0.6910823c_L$ 

The soil moisture stress is implemented as  $\beta(\theta) = \frac{\beta_0 - 1}{\theta^{*2}} (\theta - \theta^*)^2 + 1$  if  $0 \le \theta \le \theta^*$  and  $\beta(\theta) = 1$  if  $\theta > \theta^*$ .

In Stocker et al. 2020 GMD, the threshold plant-available soil water is set as  $\theta^* = 0.6 \star$  whe where whe is the site's water holding capacity. Also, the  $\beta$  reduction at low soil moisture ( $\beta_0 = \beta(0)$ ) was parameterized as a linear function of mean aridity (Eq. 20 in Stocker et al. 2020 GMD) but is considered a constant model parameter in this package. Hence, the FULL calibration setup cannot be exactly replicated.

## Value

A data frame (tibble) with one row for each site, site information stored in the nested column site\_info and outputs stored in the nested column data. See run\_pmodel\_f\_bysite for a de-tailed description of the outputs. Example outputs are provided as biomee\_p\_model\_output and biomee\_gs\_leuning\_output.

#### run\_biomee\_f\_bysite

## Examples

```
# Define model parameter values from previous work
params_modl <- list(</pre>
                     = 0.04998,
                                    # setup ORG in Stocker et al. 2020 GMD
  kphio
  kphio_par_a
                     = 0.0.
                                    # disable temperature-dependence of kphio
                     = 1.0,
  kphio_par_b
  soilm_thetastar
                     = 0.6 * 240, # old setup with soil moisture stress
                     = 0.0,
  soilm_betao
  beta_unitcostratio = 146.0,
                                    # from Atkin et al. 2015 for C3 herbaceous
  rd_to_vcmax
                     = 0.014,
  tau_acclim
                     = 30.0,
                     = 0.41
  kc_jmax
)
# Run the model for these parameters and the example drivers
output <- rsofun::runread_pmodel_f(</pre>
  drivers = rsofun::p_model_drivers,
  par = params_modl)
output_vcmax25 <- rsofun::runread_pmodel_f(</pre>
  drivers = rsofun::p_model_drivers_vcmax25,
  par = params_modl)
```

run\_biomee\_f\_bysite Run BiomeE (R wrapper)

## Description

Run BiomeE Fortran model on single site.

## Usage

```
run_biomee_f_bysite(
    sitename,
    params_siml,
    site_info,
    forcing,
    params_tile,
    params_species,
    init_cohort,
    init_soil,
    makecheck = TRUE
)
```

## Arguments

sitename	Site name.
params_siml	Simulation parameters.
site_info	Site meta info in a data.frame.

forcing	A data frame of forcing climate data, used as input.
params_tile	Tile-level model parameters, into a single row data.frame.
params_species	A data.frame containing species-specific model parameters, with one species per row. See examples biomee_gs_leuning_drivers or biomee_p_model_drivers
init_cohort	A data.frame of initial cohort specifications.
init_soil	A data.frame of initial soil pools.
makecheck	A logical specifying whether checks are performed to verify forcings and model parameters. TRUE by default.
	For further specifications of above inputs and examples see biomee_gs_leuning_drivers or biomee_p_model_drivers

## Value

Model output is provided as a list, with elements:

 $output\_hourly\_tile A data.frame containing hourly predictions$ .

year Year of the simulation. doy Day of the year. hour Hour of the day. rad Radiation, in W  $m^{-2}$ . Tair Air temperature, in Kelvin. **Prcp** Precipitation, in mm  $m^{-2}$ . **GPP** Gross primary production (kg C  $m^{-2}$  hour<sup>-1</sup>). **Resp** Plant respiration (kg C m<sup>-2</sup> hour<sup>-1</sup>). **Transp** Transpiration (mm  $m^{-2}$ ). **Evap** Evaporation (mm  $m^{-2}$ ). **Runoff** Water runoff (mm  $m^{-2}$ ). **Soilwater** Soil water content in root zone (kg  $m^{-2}$ ). wcl Volumetric soil water content for each layer (vol/vol). FLDCAP Field capacity (vol/vol). WILTPT Wilting point (vol/vol). output\_daily\_tile A data.frame with daily outputs at a tile level.

year Year of the simulation.

**doy** Day of the year.

Tc Air temperature (Kelvin).

**Prcp** Precipitation (mm  $m^{-2}$ ).

totWs Soil water content in root zone (kg  $m^{-2}$ ).

**Trsp** Transpiration (mm  $m^{2-}$ ).

**Evap** Evaporation (mm  $m^{-2}$ ).

**Runoff** Water runoff (mm  $m^{-2}$ ).

ws1 Volumetric soil water content for layer 1.

ws2 Volumetric soil water content for layer 2.

ws3 Volumetric soil water content for layer 3.

**LAI** Leaf area index  $(m^2/m^2)$ . **GPP** Gross primary production (kg C  $m^{-2}$  day<sup>-1</sup>). **Rauto** Plant autotrophic respiration (kg C m<sup>-2</sup> day<sup>-1</sup>). **Rh** Heterotrophic respiration (kg C m<sup>-2</sup> day<sup>-1</sup>). **NSC** Non-structural carbon (kg C m<sup>-2</sup>). **seed**C Biomass of seeds (kg C  $m^{-2}$ ). **leafC** Biomass of leaves (kg C  $m^{-2}$ ). **rootC** Biomass of fine roots (kg C  $m^{-2}$ ). **SW** C Biomass of sapwood (kg C  $m^{-2}$ ). **HW\_C** biomass of heartwood (kg C  $m^{-2}$ ). **NSN** Non-structural N pool (kg N  $m^{-2}$ ). seedN Nitrogen of seeds (kg N  $m^{-2}$ ). **leafN** Nitrogen of leaves (kg N  $m^{-2}$ ). **rootN** Nitrogen of roots (kg N  $m^{-2}$ ). **SW** N Nitrogen of sapwood (kg N  $m^{-2}$ ). **HW\_N** Nitrogen of heartwood (kg N  $m^{-2}$ ). **McrbC** Microbial carbon (kg C  $m^{-2}$ ). **fastSOM** Fast soil carbon pool (kg C  $m^{-2}$ ). **slowSOM** Slow soil carbon pool (kg C  $m^{-2}$ ). **McrbN** Microbial nitrogen (kg N  $m^{-2}$ ). **fastSoilN** Fast soil nitrogen pool (kg N  $m^{-2}$ ). **slowSoilN** Slow soil nitrogen pool (kg N  $m^{-2}$ ). **mineralN** Mineral nitrogen pool (kg N  $m^{-2}$ ). **N\_uptk** Nitrogen uptake (kg N m $^{-2}$ ).

output\_daily\_cohorts A data.frame with daily predictions for each canopy cohort.

year Year of the simulation.doy Day of the year.

hour Hour of the day.

**cID** An integer indicating the cohort identity.

**PFT** An integer indicating the Plant Functional Type.

layer An integer indicating the crown layer, numbered from top to bottom.

**density** Number of trees per area (trees  $ha^{-1}$ ).

f\_layer Fraction of layer area occupied by this cohort.

**LAI** Leaf area index  $(m^2/m^2)$ .

**gpp** Gross primary productivity (kg C tree<sup>-1</sup> day<sup>-1</sup>).

**resp** Plant autotrophic respiration (kg C tree<sup>-1</sup> day<sup>-1</sup>).

**transp** Transpiration (mm tree<sup>-1</sup> day<sup>-1</sup>).

**NPPleaf** Carbon allocated to leaves (kg C tree<sup>-1</sup> day<sup>-1</sup>).

**NPProof** Carbon allocated to fine roots (kg C tree<sup>-1</sup> day<sup>-1</sup>).

**NPPwood** Carbon allocated to wood (kg C tree<sup>-1</sup> day<sup>-1</sup>).

**NSC** Nonstructural carbohydrates of a tree in this cohort (kg C tree<sup>-1</sup>).

**seedC** Seed biomass of a tree in this cohort (kg C tree<sup>-1</sup>).

**leafC** Leaf biomass of a tree in this cohort (kg C tree<sup>-1</sup>). **rootC** Fine root biomass of a tree in this cohort (kg C tree<sup>-1</sup>). **SW\_C** Sapwood biomass of a tree in this cohort (kg C tree<sup>-1</sup>). **HW** C Heartwood biomass of a tree in this cohort (kg C tree<sup>-1</sup>). **NSN** Nonstructural nitrogen of a tree in this cohort (kg N tree $^{-1}$ ). seed N Seed nitrogen of a tree in this cohort (kg N tree $^{-1}$ ). **leafN** Leaf nitrogen of a tree in this cohort (kg N tree $^{-1}$ ). **rootN** Fine root nitrogen of a tree in this cohort (kg N tree $^{-1}$ ). **SW** N Sapwood nitrogen of a tree in this cohort (kg N tree<sup>-1</sup>). **HW\_N** Heartwood nitrogen of a tree in this cohort (kg N tree<sup>-1</sup>). output\_annual\_tile A data.frame with annual outputs at tile level. year Year of the simulation. **CAI** Crown area index  $(m^2/m^2)$ . **LAI** Leaf area index  $(m^2/m^2)$ . **Density** Number of trees per area (trees  $ha^{-1}$ ). **DBH** Diameter at tile level (cm). **Density12** Tree density for trees with DBH > 12 cm (individuals  $ha^{-1}$ ). **DBH12** Diameter at tile level considering trees with DBH > 12 cm (cm). QMD12 Quadratic mean diameter at tile level considering trees with DBH > 12 cm (cm). **NPP** Net primary productivity (kg C  $m^{-2}$  yr<sup>-1</sup>). **GPP** Gross primary productivity (kg C  $m^{-2}$  yr<sup>-1</sup>). **Rauto** Plant autotrophic respiration (kg C  $m^{-2}$  yr<sup>-1</sup>). **Rh** Heterotrophic respiration (kg C m<sup>-2</sup> yr<sup>-1</sup>). rain Annual precipitation (mm  $m^{-2} yr^{-1}$ ). SoilWater Soil water content in root zone (kg  $m^{-2}$ ). **Transp** Transpiration (mm m<sup>-2</sup> yr<sup>-1</sup>). **Evap** Evaporation (mm m<sup>-2</sup> vr<sup>-1</sup>). **Runoff** Water runoff (mm m<sup>-2</sup> yr<sup>-1</sup>). **plantC** Plant biomass (kg C  $m^{-2}$ ). **soilC** Soil carbon (kg C m $^{-2}$ ). **plantN** Plant nitrogen (kg N  $m^{-2}$ ). soil N Soil nitrogen (kg N  $m^{-2}$ ). totN Total nitrogen in plant and soil (kg N  $m^{-2}$ ). **NSC** Nonstructural carbohydrates (kg C  $m^{-2}$ ). **Seed**C Seed biomass (kg C  $m^{-2}$ ). **leafC** Leaf biomass (kg C  $m^{-2}$ ). **rootC** Fine root biomass (kg C  $m^{-2}$ ). **SapwoodC** Sapwood biomass (kg C  $m^{-2}$ ). **WoodC** Heartwood biomass (kg C  $m^{-2}$ ). **NSN** Nonstructural nitrogen (kg N  $m^{-2}$ ). **SeedN** Seed nitrogen (kg N  $m^{-2}$ ). **leafN** Leaf nitrogen (kg N  $m^{-2}$ ).

**rootN** Fine root nitrogen (kg N  $m^{-2}$ ). **SapwoodN** Sapwood nitrogen (kg N  $m^{-2}$ ). **WoodN** Heartwood nitrogen (kg N  $m^{-2}$ ). **McrbC** Microbial carbon (kg C  $m^{-2}$ ). **fastSOM** Fast soil carbon pool (kg C  $m^{-2}$ ). **SlowSOM** Slow soil carbon pool (kg C  $m^{-2}$ ). **McrbN** Microbial nitrogen (kg N  $m^{-2}$ ). **fastSoilN** Fast soil nitrogen pool (kg N  $m^{-2}$ ). **slowsoilN** Slow soil nitrogen pool (kg N  $m^{-2}$ ). **mineralN** Mineral nitrogen pool (kg N  $m^{-2}$ ). **N** fxed Nitrogen fixation (kg N  $m^{-2}$ ). **N\_uptk** Nitrogen uptake (kg N m $^{-2}$ ). N yrMin Annual available nitrogen (kg N  $m^{-2}$ ). **N\_P25** Annual nitrogen from plants to soil (kg N m<sup>-2</sup>). **N** loss Annual nitrogen loss (kg N m $^{-2}$ ). totseedC Total seed carbon (kg C m $^{-2}$ ). totseedN Total seed nitrogen (kg N  $m^{-2}$ ). **Seedling\_C** Total carbon from all compartments but seeds (kg C  $m^{-2}$ ). Seeling N Total nitrogen from all compartments but seeds (kg N m $^{-2}$ ). MaxAge Age of the oldest tree in the tile (years). **MaxVolume** Maximum volumne of a tree in the tile  $(m^3)$ . **MaxDBH** Maximum DBH of a tree in the tile (m). **NPPL** Growth of a tree, including carbon allocated to leaves (kg C  $m^{-2}$  year<sup>-1</sup>). **NPPW** Growth of a tree, including carbon allocated to sapwood (kg C  $m^{-2}$  year<sup>-1</sup>). **n deadtrees** Number of trees that died (trees  $m^{-2}$  year<sup>-1</sup>). **c** deadtrees Carbon biomass of trees that died (kg C  $m^{-2}$  vear<sup>-1</sup>). **m\_turnover** Continuous biomass turnover (kg C m<sup>-2</sup> year<sup>-1</sup>). c turnover time Carbon turnover rate, calculated as the ratio between plant biomass and NPP (year $^{-1}$ ). output\_annual\_cohorts A data.frame of annual outputs at the cohort level. year Year of the simulation. cID An integer indicating the cohort identity. **PFT** An integer indicating the Plant Functional Type. layer An integer indicating the crown layer, numbered from top to bottom. **density** Number of trees per area (trees  $ha^{-1}$ ). f layer Fraction of layer area occupied by this cohort. **dDBH** Diameter growth of a tree in this cohort (cm year $^{-1}$ ). **dbh** Tree diameter (cm). height Tree height (m). age Age of the cohort (years). Acrow Crown area of a tree in this cohort  $(m^2)$ .

wood Sum of sapwood and heartwood biomass of a tree in this cohort (kg C tree<sup>-1</sup>).

**nsc** Nonstructural carbohydrates in a tree (kg C tree $^{-1}$ ). **NSN** Nonstructural nitrogen of a tree (kg N tree<sup>-1</sup>). **NPPtr** Total growth of a tree, including carbon allocated to seeds, leaves, fine roots, and sapwood (kg C tree<sup>-1</sup> year<sup>-1</sup>). seed Fraction of carbon allocated to seeds to total growth. NPPL Fraction of carbon allocated to leaves to total growth. NPPR Fraction of carbon allocated to fine roots to total growth. NPPW Fraction of carbon allocated to sapwood to total growth. **GPP vr** Gross primary productivity of a tree (kg C tree<sup>-1</sup> year<sup>-1</sup>). **NPP\_yr** Net primary productivity of a tree (kg C tree<sup>-1</sup> year<sup>-1</sup>). **Rauto** Plant autotrophic respiration (kg C tree<sup>-1</sup> yr<sup>-1</sup>). **N\_uptk** Nitrogen uptake (kg N tree<sup>-1</sup> yr<sup>-1</sup>). **N** fix Nitrogen fixation (kg N tree<sup>-1</sup> yr<sup>-1</sup>). **maxLAI** Maximum leaf area index for a tree  $(m^2 m^{-2})$ . **Volume** Tree volume  $(m^3)$ . **n\_deadtrees** Number of trees that died (trees  $yr^{-1}$ ). **c\_deadtrees** Carbon biomass of trees that died (kg C yr<sup>-1</sup>). **deathrate** Mortality rate of this cohort  $(yr^{-1})$ .

#### Examples

```
# Example BiomeE model run
```

```
# Use example drivers data
drivers <- biomee_gs_leuning_drivers
# Run BiomeE for the first site
mod_output <- run_biomee_f_bysite(
   sitename = drivers$sitename[1],</pre>
```

```
params_siml = drivers$params_siml[[1]],
site_info = drivers$params_siml[[1]],
forcing = drivers$forcing[[1]],
params_tile = drivers$params_tile[[1]],
params_species = drivers$params_species[[1]],
init_cohort = drivers$init_cohort[[1]],
init_soil = drivers$init_soil[[1]]
```

run\_pmodel\_f\_bysite Run P-model (R wrapper)

## Description

Run P-model Fortran model on single site.

run\_pmodel\_f\_bysite

## Usage

```
run_pmodel_f_bysite(
    sitename,
    params_siml,
    site_info,
    forcing,
    params_modl,
    makecheck = TRUE,
    verbose = TRUE
)
```

# Arguments

sitename	Site name.
params_siml	Simulation parameters.
site_info	Site meta info in a data.frame.
forcing	A data frame of forcing climate data, used as input.
params_modl	A named list of free (calibratable) model parameters. See runread_pmodel_f
makecheck	A logical specifying whether checks are performed to verify forcings and model parameters. TRUE by default.
verbose	A logical specifying whether to print warnings. Defaults to TRUE.
	For further specifications of above inputs and examples see p_model_drivers or p_model_drivers_vcmax25

## Details

Depending on the input model parameters, it's possible to run the different P-model setups presented in Stocker et al. 2020 GMD. The P-model version implemented in this package allows more flexibility than the one presented in the paper, with the following functions:

The temperature dependence of the quantum yield efficiency is given by:

$$\varphi_0(T) = c(1 + a(T - b)^2) \text{ if } 0 < c(1 + a(T - b)^2) < 1, \\
\varphi_0(T) = 0 \text{ if } c(1 + a(T - b)^2) \le 0, \text{ and} \\
\varphi_0(T) = 1 \text{ if } c(1 + a(T - b)^2) \ge 1.$$

The ORG setup can be reproduced by setting kphio\_par\_a = 0 and calibrating the kphio parameter only. The BRC setup (which calibrates  $c_L = \frac{a_L b_L}{4}$  in Eq. 18) is more difficult to reproduce, since the temperature-dependency has been reformulated and a custom cost function would be necessary for calibration. The new parameters are related to  $c_L$  as follows:

```
a = -0.0004919819

b = 32.35294

c = 0.6910823c_L
```

The soil moisture stress is implemented as

$$\beta(\theta) = \frac{\beta_0 - 1}{\theta^{*2}} (\theta - \theta^*)^2 + 1 \text{ if } 0 \le \theta \le \theta^* \text{ and } \beta(\theta) = 1 \text{ if } \theta > \theta^*.$$

In Stocker et al. 2020 GMD, the threshold plant-available soil water is set as  $\theta^* = 0.6 \star$  whe where whe is the site's water holding capacity. Also, the  $\beta$  reduction at low soil moisture ( $\beta_0 = \beta(0)$ ) was parameterized as a linear function of mean aridity (Eq. 20 in Stocker et al. 2020 GMD) but is

considered a constant model parameter in this package. Hence, the FULL calibration setup cannot be exactly replicated.

#### Value

Model output is provided as a tidy dataframe, with columns:

- date Date of the observation in YYYY-MM-DD format.
- year\_dec Decimal representation of year and day of the year (for example, 2007.000 corresponds to 2007-01-01 and 2007.003 to 2007-01-02.
- fapar Fraction of photosynthetic active radiation (fAPAR), taking values between 0 and 1.
- gpp Gross Primary Productivity (GPP) for each time stamp (in gC m<sup>-2</sup> d<sup>-1</sup>).
- aet Actual evapotranspiration (AET), calculated by SPLASH following Priestly-Taylor (in mm  $d^{-1}$ ).
- le Latent heat flux (in J m<sup>-2</sup> d<sup>-1</sup>).
- pet Potential evapotranspiration (PET), calculated by SPLASH following Priestly-Taylor (in mm  $d^{-1}$ ).
- vcmax Maximum rate of RuBisCO carboxylation (Vcmax) (in mol C m<sup>-2</sup> d<sup>-1</sup>).
- jmax Maximum rate of electron transport for RuBP regeneration (in mol  $CO_2 \text{ m}^{-2} \text{ s}^{-1}$ ).
- vcmax25 Maximum rate of carboxylation (Vcmax), normalised to  $25^{\circ}$ C (in mol C m<sup>-2</sup> d<sup>-1</sup>).

jmax25 Maximum rate of electron transport, normalised to  $25^{\circ}$ C (in mol C m<sup>-2</sup> s<sup>-1</sup>).

gs\_accl Acclimated stomatal conductance (in mol C m<sup>-2</sup> d<sup>-1</sup> Pa<sup>-1</sup>).

- wscal Relative soil water content, between 0 (permanent wilting point, PWP) and 1 (field capacity, FC).
- chi Ratio of leaf-internal to ambient CO<sub>2</sub>, ci:ca (unitless).
- iwue Intrinsic water use efficiency (iWUE) (in Pa).
- rd Dark respiration (Rd) in gC m<sup>-2</sup> d<sup>-1</sup>.
- tsoil Soil temperature, in <sup>o</sup>C.
- netrad Net radiation, in W m<sup>-2</sup>. WARNING: this is currently ignored as a model forcing. Instead, net radiation is internally calculated by SPLASH.

wcont Soil water content, in mm.

- snow Snow water equivalents, in mm.
- cond Water input by condensation, in mm  $d^{-1}$

## Examples

```
# Define model parameter values from previous work
params_modl <- list(
   kphio = 0.04998, # setup ORG in Stocker et al. 2020 GMD
   kphio_par_a = 0.0, # disable temperature-dependence of kphio
   kphio_par_b = 1.0,
   soilm_thetastar = 0.6 * 240, # old setup with soil moisture stress
   soilm_betao = 0.0,
   beta_unitcostratio = 146.0,</pre>
```

```
rd_to_vcmax = 0.014, # from Atkin et al. 2015 for C3 herbaceous
tau_acclim = 30.0,
kc_jmax = 0.41
)
# Run the Fortran P-model
mod_output <- run_pmodel_f_bysite(
    # unnest drivers example data
    sitename = p_model_drivers$sitename[1],
    params_siml = p_model_drivers$params_siml[[1]],
    site_info = p_model_drivers$params_siml[[1]],
    forcing = p_model_drivers$forcing[[1]],
    params_modl = params_modl
)
```

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