

Package ‘csmbuilder’

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Type Package

Title A Collection of Tools for Building Cropping System Models

Version 0.1.1

Description A collection of tools for designing, implementing, testing, documenting and visualizing dynamic simulation cropping system models. Models are specified as a combination of state variables, parameters, intermediate factors and input data that define a system of ordinary differential equations. Specified models can be used to simulate dynamic processes using numerical integration algorithms.

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Depends R (>= 4.2.0)

Suggests deSolve, Rcpp, tinytest

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URL <https://github.com/palderman/csmbuilder>

BugReports <https://github.com/palderman/csmbuilder/issues>

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csm_arr_fr_active	<i>Fraction of active enzymes based on modified Arrhenius function</i>
-------------------	--

Description

This function computes the fraction of active enzymes according to the the modified Arrhenius function. The fraction of denatured enzymes can be calculated by subtracting this function from 1.

Usage

```
csm_arr_fr_active(Tt, H, E, To)
```

Arguments

Tt	temperature in Celsius
H	deactivation energy parameter
E	activation energy parameter
To	optimum temperature in Celsius

Value

a numeric value of the fraction of active enzymes rate at temperature Tt

`csm_create_data_structure`*Create a cropping systems model (CSM) data structure*

Description

Create a cropping systems model (CSM) data structure

Usage

```
csm_create_data_structure(name, definition, variables, n_dim = 1)
```

Arguments

<code>name</code>	a length-one character vector name of a variable
<code>definition</code>	the definition of the data structure
<code>variables</code>	a list of the CSM variables (as defined with <code>[csmbuilder::csm_create_variable()]</code>) that are contained within the data structure
<code>n_dim</code>	the number of dimensions in the data structure; default value of 1 (i.e. each variable is expected to be a scalar value)

Value

a list of 'csm_data_structure' objects

Examples

```
# Create variables:
wth_variables <- c(
  csm_create_variable("time",
                      "time of observation",
                      "days"),
  csm_create_variable("Tair",
                      "air temperature",
                      "Celsius"),
  csm_create_variable("SRAD",
                      "solar radiation",
                      "MJ/m2/d"))

# Create weather data structure:
weather <- csm_create_data_structure("weather",
                                     "weather data",
                                     wth_variables,
                                     n_dim = 2)
```

csm_create_model	<i>Create a model definition for a Cropping System Model (CSM)</i>
------------------	--

Description

Create a model definition for a Cropping System Model (CSM)

Usage

```
csm_create_model(state, ..., name = "model")
```

Arguments

state	a list vector containing CSM state variables defined using csm_create_state() in the intended order
...	optional arguments of list vectors containing CSM parameters defined using csm_create_parameter() or CSM variables defined using csm_create_variable()
name	a character string containing a name for the models

Value

a list which defines all components of a model including state variables, input variables, parameters, transformed variables and data structures.

Examples

```
# Define state variables
lv_state <- csm_create_state(
  c("x", "y"),
  definition = c("prey", "predator"),
  units = c("rabbits per square km", "foxes per square km"),
  expression(~alpha*x-beta*x*y, ~delta*x*y-gamma*y))

# Define parameters
lv_parameters <- csm_create_parameter(
  c("alpha", "beta", "gamma", "delta"),
  definition = c("maximum prey per capita growth rate",
    "effect of predator population on prey death rate",
    "predator per capita death rate",
    "effect of prey population on predator growth rate"),
  units = c("rabbits per rabbit", "per fox",
    "foxes per fox", "foxes per rabbit"))

# Define model
lotka_volterra_model <-
  csm_create_model(
    state = lv_state,
    parms = lv_parameters)
```

`csm_create_parameter` *Create a cropping systems model (CSM) parameter variable*

Description

Create a cropping systems model (CSM) parameter variable

Usage

```
csm_create_parameter(
  name,
  definition,
  units,
  lower_bound = NULL,
  upper_bound = NULL
)
```

Arguments

<code>name</code>	a length-one character vector name of a variable
<code>definition</code>	a length-one character vector that defines the CSM variable
<code>units</code>	a length-one character vector of the units of the CSM variable
<code>lower_bound</code>	a numerical value providing the lower bound for the parameter
<code>upper_bound</code>	a numerical value providing the upper bound for the parameter

Value

a list of `csm_parameter` objects

Examples

```
# Define Lotka-Volterra parameters with single call

lv_parameters <- csm_create_parameter(
  name = c("alpha", "beta", "gamma", "delta"),
  definition = c("maximum prey per capita growth rate",
    "effect of predator population on prey death rate",
    "predator per capita death rate",
    "effect of prey population on predator growth rate"),
  units = c("rabbits per rabbit", "per fox",
    "foxes per fox", "foxes per rabbit"))

# Define Lotka-Volterra parameters with multiple calls

lv_parameters <-
  c(
    csm_create_parameter(
```

```

    name = "alpha",
    definition = "maximum prey per capita growth rate",
    units = "rabbits per rabbit"),
csm_create_parameter(
  name = "beta",
  definition = "effect of predator population on prey death rate",
  units = "per fox"),
csm_create_parameter(
  name = "gamma",
  definition = "predator per capita death rate",
  units = "foxes per fox"),
csm_create_parameter(
  name = "delta",
  definition = "effect of prey population on predator growth rate",
  units = "foxes per rabbit"))

```

csm_create_state	<i>Create a cropping systems model (CSM) state variable</i>
------------------	---

Description

Create a cropping systems model (CSM) state variable

Usage

```
csm_create_state(name, definition, units, equation)
```

Arguments

name	a length-one character vector name of a variable
definition	a length-one character vector that defines the CSM variable
units	a length-one character vector of the units of the CSM variable
equation	an R expression with the equation for the rate of change of the CSM state variable

Value

a list of csm_state objects

Examples

```

# Define state variables with single call

lv_state <- csm_create_state(
  c("x", "y"),
  definition = c("prey", "predator"),
  units = c("rabbits per square km", "foxes per square km"),

```

```

    expression(~alpha*x-beta*x*y, ~delta*x*y-gamma*y))

# Define state variables with multiple calls

lv_state <-
c(
  csm_create_state(
    name = "x",
    definition = "prey",
    units = "rabbits per square km",
    equation = ~alpha*x-beta*x*y),
  csm_create_state(
    name = "y",
    definition = "predator",
    units = "foxes per square km",
    equation = ~delta*x*y-gamma*y)
)

```

csm_create_transform *Create a cropping systems model (CSM) transformed variable*

Description

Create a cropping systems model (CSM) transformed variable

Usage

```
csm_create_transform(name, definition, units, equation)
```

Arguments

name	a length-one character vector name of a variable
definition	a length-one character vector that defines the CSM variable
units	a length-one character vector of the units of the CSM variable
equation	an R expression with the equation for the value of the transformed CSM state variable

Value

a list of csm_transform objects

Examples

```

# Define intermediate factor

sp_factors <- csmbuilder::csm_create_transform(
  name = "fv",

```

```
definition = "vernalization factor",
units = "relative progress towards complete vernalization (0-1)",
equation = ~min(c(cum_vrn/vreq, 1)))
```

`csm_create_variable` *Create a cropping systems model (CSM) variable*

Description

Create a cropping systems model (CSM) variable

Usage

```
csm_create_variable(name, definition, units)
```

Arguments

<code>name</code>	a length-one character vector name of a variable
<code>definition</code>	a length-one character vector that defines the CSM variable
<code>units</code>	a length-one character vector of the units of the CSM variable

Value

a list of `csm_variable` objects

Examples

```
Tair <- csm_create_variable(name = "Tair",
                           definition = "air temperature",
                           units = "Celsius")
```

`csm_get_at_t` *Linearly interpolate a time-varying variable at specific time point*

Description

Linearly interpolate a time-varying variable at specific time point

Usage

```
csm_get_at_t(
  x,
  t_ind,
  t,
  method = "linear",
  search = c("interpolation", "bisection", "brute force", "i=t+1")
)
```

Arguments

x	a vector of a time-varying values for which to interpolate
t_ind	a vector of times corresponding to the values in x
t	a single time point at which to return a value
method	a string indicating what method to use for interpolation. One of: "linear"
search	a string indicating what method to use for finding the correct indices within t_ind. One of: "bisection", "interpolation"

Value

the numeric value of the time-varying variable interpolated at time t

csm_hill_down_reg	<i>Hill equation for down-regulation</i>
-------------------	--

Description

Hill equation for down-regulation

Usage

```
csm_hill_down_reg(L, K, n)
```

Arguments

L	a numeric value providing the ligand concentration
K	a numeric value providing the ligand concentration at half occupation
n	a numeric value providing the Hill coefficient

Value

a numeric value between 0 and 1

csm_hill_up_reg	<i>Hill equation for up-regulation</i>
-----------------	--

Description

Hill equation for up-regulation

Usage

csm_hill_up_reg(L, K, n)

Arguments

L	a numeric value providing the ligand concentration
K	a numeric value providing the ligand concentration at half occupation
n	a numeric value providing the Hill coefficient

Value

a numeric value between 0 and 1

csm_mod_arr	<i>Modified Arrhenius function</i>
-------------	------------------------------------

Description

Modified Arrhenius function

Usage

csm_mod_arr(Tt, ko, H, E, To)

Arguments

Tt	temperature in Celsius
ko	reaction rate at the optimum temperature (To)
H	deactivation energy parameter
E	activation energy parameter
To	optimum temperature in Celsius

Value

a numeric value of the reaction rate at temperature Tt

csm_render_model	<i>Render a defined Cropping System Model (CSM)</i>
------------------	---

Description

Render a defined Cropping System Model (CSM)

Usage

```
csm_render_model(
  model,
  name = "dy_dt",
  output_type = c("function", "code"),
  language = c("R", "Rcpp"),
  arg_alias = NULL,
  insert_functions = NULL
)
```

Arguments

model	a list vector containing a CSM as created by csm_create_model()
name	name of the resulting function
output_type	a character value indicating the type of output to produce; one of: "function" (a callable function) or "code" (computer code for the model)
language	a character value indicating which programming language into which to render the model
arg_alias	an optional named character vector whose names indicate variables for which to use an alias within the generated function and whose elements provide the corresponding alias
insert_functions	an optional list of functions to add to rendered code

Value

Either an R function object (if output_type="function") or a character vector of model code (if output_type="code") in the programming language specified by language.

Examples

```
# Define state variables
lv_state <- csm_create_state(
  c("x", "y"),
  definition = c("prey", "predator"),
  units = c("rabbits per square km", "foxes per square km"),
  expression(~alpha*x-beta*x*y, ~delta*x*y-gamma*y))
```

```

# Define parameters
lv_parameters <- csm_create_parameter(
  c("alpha", "beta", "gamma", "delta"),
  definition = c("maximum prey per capita growth rate",
    "effect of predator population on prey death rate",
    "predator per capita death rate",
    "effect of prey population on predator growth rate"),
  units = c("rabbits per rabbit", "per fox",
    "foxes per fox", "foxes per rabbit"))

# Define model
lotka_volterra_model <-
  csm_create_model(
    state = lv_state,
    parms = lv_parameters)

# Render model into raw R code
lotka_volterra_code <-
  csm_render_model(lotka_volterra_model,
    output_type = "code",
    language = "R")

# Render model into a callable R function
lotka_volterra_fun <-
  csm_render_model(lotka_volterra_model,
    output_type = "function",
    language = "R")

```

csm_run_sim

Run a Cropping System Model (CSM) simulation

Description

Run a Cropping System Model (CSM) simulation

Usage

```
csm_run_sim(model_function, y_init, t, ..., method = "euler")
```

Arguments

model_function	a rendered model produced by csm_render_model()
y_init	a vector of initial values for the model state variables
t	an optional vector of time points for which simulated model outputs are desired
...	additional arguments to pass to model_function for simulation
method	numerical integration method to be used. See deSolve::ode() for more details

Value

a data frame with one row for each time point specified by t

Examples

```
# Define state variables
lv_state <- csm_create_state(
  c("x", "y"),
  definition = c("prey", "predator"),
  units = c("rabbits per square km", "foxes per square km"),
  expression(~alpha*x-beta*x*y, ~delta*x*y-gamma*y))

# Define parameters
lv_parameters <- csm_create_parameter(
  c("alpha", "beta", "gamma", "delta"),
  definition = c("maximum prey per capita growth rate",
    "effect of predator population on prey death rate",
    "predator per capita death rate",
    "effect of prey population on predator growth rate"),
  units = c("rabbits per rabbit", "per fox",
    "foxes per fox", "foxes per rabbit"))

# Define model
lotka_volterra_model <-
  csm_create_model(
    state = lv_state,
    parms = lv_parameters)

# Render model into a callable R function
lotka_volterra_fun <-
  csm_render_model(lotka_volterra_model,
    output_type = "function",
    language = "R")

# Run model simulation
lotka_volterra_out <-
  csm_run_sim(model_function = lotka_volterra_fun,
    y_init = c(x = 10,
      y = 10),
    t = csm_time_vector(0, 100, 0.01),
    parms = c(alpha = 1.1,
      beta = 0.4,
      gamma = 0.1,
      delta = 0.4))
```

Description

Run a group of Cropping System Model (CSM) simulations

Usage

```
csm_run_sim_group(
  model_function,
  y_init,
  t,
  ...,
  method = "euler",
  return_df = TRUE
)
```

Arguments

<code>model_function</code>	a rendered model produced by csm_render_model()
<code>y_init</code>	a list of vectors of initial values for the model state variables. To use the same initial conditions for all simulation group members, the list should be of length one. Otherwise, the length of the list should correspond to the number of simulation group members.
<code>t</code>	an optional list of vectors of time points for which simulated model outputs are desired. To use the same time points for all simulation group members, the list should be of length one. Otherwise, the length of the list should correspond to the number of simulation group members.
<code>...</code>	additional arguments to pass to <code>model_function</code> for simulation. Each argument should be supplied as a list. To use the same argument value for all simulation group members, the list should be of length one. Otherwise, the length of the list should correspond to the number of simulation group members.
<code>method</code>	numerical integration method to be used. See deSolve::ode() for more details
<code>return_df</code>	a logical value with a default value of TRUE that indicates whether to return output as a data frame (if set to TRUE) or as a list (if set to FALSE).

Value

If `return_df` is set to TRUE, the function returns a data frame with one row for each time point specified by `t` within each simulation group member. The simulation group member is indicated by a column within the data frame (`sim_no`). If `return_df` is set to FALSE, the function returns a list of data frames, each of which is the output of a simulation group member and includes one row for each time point specified by `t`

Examples

```
# Define state variables
lv_state <- csm_create_state(
  c("x", "y"),
  definition = c("prey", "predator"),
  units = c("rabbits per square km", "foxes per square km"),
```

```

expression(~alpha*x-beta*x*y, ~delta*x*y-gamma*y))

# Define parameters
lv_parameters <- csm_create_parameter(
  c("alpha", "beta", "gamma", "delta"),
  definition = c("maximum prey per capita growth rate",
    "effect of predator population on prey death rate",
    "predator per capita death rate",
    "effect of prey population on predator growth rate"),
  units = c("rabbits per rabbit", "per fox",
    "foxes per fox", "foxes per rabbit"))

# Define model
lotka_volterra_model <-
  csm_create_model(
    state = lv_state,
    parms = lv_parameters)

# Render model into a callable R function
lotka_volterra_fun <-
  csm_render_model(lotka_volterra_model,
    output_type = "function",
    language = "R")

# Run model simulations for two parameter vectors
lotka_volterra_out <-
  csm_run_sim_group(model_function = lotka_volterra_fun,
    y_init = list(c(x = 10,
      y = 10)),
    t = list(csm_time_vector(0, 100, 0.01)),
    parms = list(c(alpha = 1.1,
      beta = 0.4,
      gamma = 0.1,
      delta = 0.4),
      c(alpha = 1.2,
        beta = 0.5,
        gamma = 0.15,
        delta = 0.35)))

```

csm_time_vector

Generate vector of times for simulation

Description

Generate vector of times for simulation

Usage

```
csm_time_vector(t_init, t_max, dt = 1)
```

Arguments

t_init	a numerical value providing the initial time to use for simulation
t_max	a numerical value providing the final time to use for simulation
dt	a numerical value providing the size of the time step to use for simulation

Value

a numeric vector

Examples

```
csm_time_vector(0, 100, dt = 0.01)
```

is_data_structure	<i>Determine if object is a data structure</i>
-------------------	--

Description

Determine if object is a data structure

Usage

```
is_data_structure(x)
```

Arguments

x	any R object
---	--------------

Value

a logical value indicating whether or not x is of class csm_data_structure

is_input	<i>Determine if object is a model input</i>
----------	---

Description

Determine if object is a model input

Usage

```
is_input(x)
```

Arguments

x	any R object
---	--------------

Value

a logical value indicating whether or not x is an input variable

is_parameter	<i>Determine if object is a model parameter</i>
--------------	---

Description

Determine if object is a model parameter

Usage

```
is_parameter(x)
```

Arguments

x	any R object
---	--------------

Value

a logical value indicating whether or not x is of class csm_parameter

is_state_variable	<i>Determine if object is state variable</i>
-------------------	--

Description

Determine if object is state variable

Usage

```
is_state_variable(x)
```

Arguments

x	any R object
---	--------------

Value

a logical value indicating whether or not x is of class csm_state

is_transform	<i>Determine if object is a transformed variable</i>
--------------	--

Description

Determine if object is a transformed variable

Usage

```
is_transform(x)
```

Arguments

x	any R object
---	--------------

Value

a logical value indicating whether or not x is of class csm_transform

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