Package 'odin'

October 14, 2022

Title ODE Generation and Integration

Version 1.2.4

Description Generate systems of ordinary differential equations (ODE) and integrate them, using a domain specific language (DSL). The DSL uses R's syntax, but compiles to C in order to efficiently solve the system. A solver is not provided, but instead interfaces to the packages 'deSolve' and 'dde' are generated. With these, while solving the differential equations, no allocations are done and the calculations remain entirely in compiled code. Alternatively, a model can be transpiled to R for use in contexts where a C compiler is not present. After compilation, models can be inspected to return information about parameters and outputs, or intermediate values after calculations. 'odin' is not targeted at any particular domain and is suitable for any system that can be expressed primarily as mathematical expressions. Additional support is provided for working with delays (delay differential equations, DDE), using interpolated functions during interpolation, and for integrating quantities that represent arrays.

License MIT + file LICENSE

URL https://github.com/mrc-ide/odin

BugReports https://github.com/mrc-ide/odin/issues

Imports R6, cinterpolate (>= 1.0.0), deSolve, digest, glue, jsonlite, ring, withr

Suggests dde (>= 1.0.0), jsonvalidate (>= 1.1.0), knitr, mockery, pkgbuild, pkgload, rlang, rmarkdown, testthat

VignetteBuilder knitr

RoxygenNote 7.1.1

Encoding UTF-8

Language en-GB

NeedsCompilation no

2 can_compile

Author Rich FitzJohn [aut, cre], Thibaut Jombart [ctb], Imperial College of Science, Technology and Medicine [cph] Maintainer Rich FitzJohn < rich.fitzjohn@gmail.com> Repository CRAN

Date/Publication 2022-04-28 08:50:02 UTC

R topics documented:

Index		13
	odin_validate	 11
	odin_package	 9
	odin_ir_deserialise	 7
	odin_ir	 ϵ
	can compile	 2

Test if compilation is possible

Description

Test if compilation appears possible. This is used in some examples, and tries compiling a trivial C program with pkgbuild. Results are cached between runs within a session so this should be fast to rely on.

Usage

```
can_compile(verbose = FALSE, refresh = FALSE)
```

Arguments

Be verbose when running commands? verbose

refresh Try again to compile, skipping the cached value?

Details

We use pkgbuild in order to build packages, and it includes a set of heuristics to locate and organise your C compiler. The most likely people affected here are Windows users; if you get this ensure that you have rools installed. Using pkgbuild::find_rtools() with debug = TRUE may be helpful for diagnosing compiler issues.

odin 3

Value

A logical scalar

Examples

```
can_compile() # will take ~0.1s the first time
can_compile() # should be basically instantaneous
```

odin

Create an odin model

Description

Create an odin model from a file, text string(s) or expression. The odin_ version is a "standard evaluation" escape hatch.

Usage

```
odin(x, verbose = NULL, target = NULL, workdir = NULL, validate = NULL,
    pretty = NULL, skip_cache = NULL, compiler_warnings = NULL,
    no_check_unused_equations = NULL, options = NULL)

odin_(x, verbose = NULL, target = NULL, workdir = NULL,
    validate = NULL, pretty = NULL, skip_cache = NULL,
    compiler_warnings = NULL, no_check_unused_equations = NULL,
    options = NULL)
```

Arguments

х	Either the name of a file to read, a text string (if length is greater than 1 elements will be joined with newlines) or an expression.
verbose	Logical scalar indicating if the compilation should be verbose. Defaults to the value of the option odin.verbose or FALSE otherwise.
target	Compilation target. Options are "c" and "r", defaulting to the option odin.target or "c" otherwise.
workdir	Directory to use for any generated files. This is only relevant for the "c" target. Defaults to the value of the option odin.workdir or tempdir() otherwise.
validate	Validate the model's intermediate representation against the included schema. Normally this is not needed and is intended primarily for development use. Defaults to the value of the option odin.validate or FALSE otherwise.
pretty	Pretty-print the model's intermediate representation. Normally this is not needed and is intended primarily for development use. Defaults to the value of the option odin.pretty or FALSE otherwise.
skip_cache	Skip odin's cache. This might be useful if the model appears not to compile when you would expect it to. Hopefully this will not be needed often. Defaults to the option odin.skip_cache or FALSE otherwise.

4 odin

compiler_warnings

Previously this attempted detection of compiler warnings (with some degree of success), but is currently ignored. This may become supported again in a future version depending on underlying support in pkgbuild.

no_check_unused_equations

If TRUE, then don't print messages about unused variables. Defaults to the option odin.no_check_unused_equations or FALSE otherwise.

options

Named list of options. If provided, then all other options are ignored.

Details

Do not use odin::odin in a package; you almost certainly want to use odin_package instead.

A generated model can return information about itself; odin_ir

Value

An odin_generator object (an R6 class) which can be used to create model instances.

User parameters

If the model accepts user parameters, then the parameter to the constructor or the \$set_user() method can be used to control the behaviour when unknown user actions are passed into the model. Possible values are the strings stop (throw an error), warning (issue a warning but keep going), message (print a message and keep going) or ignore (do nothing). Defaults to the option odin.unused_user_action, or warning otherwise.

Delay equations with dde

When generating a model one must chose between using the dde package to solve the system or the default deSolve. Future versions may allow this to switch when using run, but for now this requires tweaking the generated code to a point where one must decide at generation. dde implements only the Dormand-Prince 5th order dense output solver, with a delay equation solver that may perform better than the solvers in deSolve. For non-delay equations, deSolve is very likely to outperform the simple solver implemented.

Author(s)

Rich FitzJohn

Examples

```
## Compile the model; exp_decay here is an R6ClassGenerator and will
## generate instances of a model of exponential decay:
exp_decay <- odin::odin({
  deriv(y) <- -0.5 * y
  initial(y) <- 1
}, target = "r")
## Generate an instance; there are no parameters here so all instances
## are the same and this looks a bit pointless. But this step is</pre>
```

odin_build 5

```
## required because in general you don't want to have to compile the
## model every time it is used (so the generator will go in a
## package).
mod <- exp_decay$new()

## Run the model for a series of times from 0 to 10:
t <- seq(0, 10, length.out = 101)
y <- mod$run(t)
plot(y, xlab = "Time", ylab = "y", main = "", las = 1)</pre>
```

odin_build

Build an odin model generator from its IR

Description

Build an odin model generator from its intermediate representation, as generated by odin_parse. This function is for advanced use.

Usage

```
odin_build(x, options = NULL)
```

Arguments

x An odin ir (json) object or output from odin_validate.

options Options to pass to the build stage (see odin_options

Details

In applications that want to inspect the intermediate representation rather before compiling, rather than directly using odin, use either odin_parse or odin_validate and then pass the result to odin::odin_build.

The return value of this function includes information about how long the compilation took, if it was successful, etc, in the same style as odin_validate:

success Logical, indicating if compilation was successful

elapsed Time taken to compile the model, as a proc_time object, as returned by proc.time.

output Any output produced when compiling the model (only present if compiling to C, and if the cache was not hit.

model The model itself, as an odin_generator object, as returned by odin.

ir The intermediate representation.

error Any error thrown during compilation

See Also

odin_parse, which creates intermediate representations used by this function.

odin_ir

Examples

```
# Parse a model of exponential decay
ir <- odin::odin_parse({
    deriv(y) <- -0.5 * y
    initial(y) <- 1
})

# Compile the model:
options <- odin::odin_options(target = "r")
res <- odin::odin_build(ir, options)

# All results:
res

# The model:
mod <- res$model$new()
mod$run(0:10)</pre>
```

odin_ir

Return detailed information about an odin model

Description

Return detailed information about an odin model. This is the mechanism through which coef works with odin.

Usage

```
odin_ir(x, parsed = FALSE)
```

Arguments

x An odin_generator function, as created by odin::odin

parsed Logical, indicating if the representation should be parsed and converted into an

R object. If FALSE we return a json string.

Warning

The returned data is subject to change for a few versions while I work out how we'll use it.

Examples

```
exp_decay <- odin::odin({
  deriv(y) <- -0.5 * y
  initial(y) <- 1
}, target = "r")
odin::odin_ir(exp_decay)
coef(exp_decay)</pre>
```

odin_ir_deserialise 7

odin_ir_deserialise

Deserialise odin's IR

Description

Deserialise odin's intermediate model representation from a json string into an R object. Unlike the json, there is no schema for this representation. This function provides access to the same deserialisation that odin uses internally so may be useful in applications.

Usage

```
odin_ir_deserialise(x)
```

Arguments

Χ

An intermediate representation as a json string

Value

A named list

See Also

odin_parse

Examples

```
# Parse a model of exponential decay
ir <- odin::odin_parse({
   deriv(y) <- -0.5 * y
   initial(y) <- 1
})
# Convert the representation to an R object
odin::odin_ir_deserialise(ir)</pre>
```

odin_options

Odin options

Description

For lower-level odin functions odin_parse, odin_validate we only accept a list of options rather than individually named options.

8 odin_options

Usage

```
odin_options(verbose = NULL, target = NULL, workdir = NULL,
  validate = NULL, pretty = NULL, skip_cache = NULL,
  compiler_warnings = NULL, no_check_unused_equations = NULL,
  rewrite_dims = NULL, rewrite_constants = NULL, substitutions = NULL,
  options = NULL)
```

Arguments

verbose Logical scalar indicating if the compilation should be verbose. Defaults to the

value of the option odin. verbose or FALSE otherwise.

target Compilation target. Options are "c" and "r", defaulting to the option odin.target

or "c" otherwise.

workdir Directory to use for any generated files. This is only relevant for the "c" target.

Defaults to the value of the option odin.workdir or tempdir() otherwise.

validate Validate the model's intermediate representation against the included schema.

Normally this is not needed and is intended primarily for development use. De-

faults to the value of the option odin. validate or FALSE otherwise.

Pretty-print the model's intermediate representation. Normally this is not needed

and is intended primarily for development use. Defaults to the value of the

option odin.pretty or FALSE otherwise.

skip_cache Skip odin's cache. This might be useful if the model appears not to compile

when you would expect it to. Hopefully this will not be needed often. Defaults

to the option odin. skip_cache or FALSE otherwise.

compiler_warnings

Previously this attempted detection of compiler warnings (with some degree of success), but is currently ignored. This may become supported again in a future

version depending on underlying support in pkgbuild.

no_check_unused_equations

If TRUE, then don't print messages about unused variables. Defaults to the option

odin.no_check_unused_equations or FALSE otherwise.

ing arrays). If TRUE then we replace dimensions known at compile-time with literal integers, and those known at initialisation with simplified and shared expressions. You may get less-comprehensible error messages with this option set to TRUE because parts of the model have been effectively evaluated during

processing.

rewrite_constants

Logical, indicating if odin should try and rewrite *all* constant scalars. This is a superset of rewrite_dims and may be slow for large models. Doing this will make your model less debuggable; error messages will reference expressions that have been extensively rewritten, some variables will have been removed entirely or merged with other identical expressions, and the generated code may not be obviously connected to the original code.

odin_package 9

substitutions Optionally, a list of values to substitute into model specification as constants,

even though they are declared as user(). This will be most useful in conjunction with rewrite_dims to create a copy of your model with dimensions known at

compile time and all loops using literal integers.

options Named list of options. If provided, then all other options are ignored.

Value

A list of parameters, of class odin_options

Examples

odin_options()

odin_package

Create odin model in a package

Description

Create an odin model within an existing package.

Usage

```
odin_package(path_package)
```

Arguments

path_package Path to the package root (the directory that contains DESCRIPTION)

Details

I am resisting the urge to actually create the package here. There are better options than I can come up with; for example devtools::create, pkgkitten::kitten, mason::mason, or creating DESCRIPTION files using desc. What is required here is that your package:

- Lists odin in Imports:
- Includes useDynLib(<your package name>) in NAMESPACE (possibly via a roxygen comment @useDynLib <your package name>
- To avoid a NOTE in R CMD check, import something from odin in your namespace (e.g., importFrom("odin", "odin")s or roxygen @importFrom(odin, odin)

Point this function at the package root (the directory containing DESCRIPTION and it will write out files src/odin.c and odin.R. These files will be overwritten without warning by running this again.

10 odin_parse

Examples

```
path <- tempfile()
dir.create(path)

src <- system.file("examples/package", package = "odin", mustWork = TRUE)
file.copy(src, path, recursive = TRUE)
pkg <- file.path(path, "package")

# The package is minimal:
dir(pkg)

# But contains odin files in inst/odin
dir(file.path(pkg, "inst/odin"))

# Compile the odin code in the package
odin::odin_package(pkg)

# Which creates the rest of the package structure
dir(pkg)
dir(file.path(pkg, "R"))
dir(file.path(pkg, "src"))</pre>
```

odin_parse

Parse an odin model

Description

Parse an odin model, returning an intermediate representation. The odin_parse_ version is a "standard evaluation" escape hatch.

Usage

```
odin_parse(x, type = NULL, options = NULL)
odin_parse_(x, options = NULL, type = NULL)
```

Arguments

type

x An expression, character vector or filename with the odin code

An optional string indicating the the type of input - must be one of expression, file or text if provided. This skips the type detection code used by odin and

makes validating user input easier.

options odin options; see odin_options. The primary options that affect the parse stage

are validate and pretty.

Details

A schema for the intermediate representation is available in the package as schema.json. It is subject to change at this point.

odin_validate 11

See Also

odin_validate, which wraps this function where parsing might fail, and odin_build for building odin models from an intermediate representation.

Examples

```
# Parse a model of exponential decay
ir <- odin::odin_parse({
    deriv(y) <- -0.5 * y
    initial(y) <- 1
})

# This is odin's intermediate representation of the model
ir

# If parsing odin models programmatically, it is better to use
# odin_parse_; construct the model as a string, from a file, or as a
# quoted expression:
code <- quote({
    deriv(y) <- -0.5 * y
    initial(y) <- 1
})

odin::odin_parse_(code)</pre>
```

odin_validate

Validate an odin model

Description

Validate an odin model. This function is closer to odin_parse_ than odin_parse because it does not do any quoting of the code. It is primarily intended for use within other applications.

Usage

```
odin_validate(x, type = NULL, options = NULL)
```

Arguments

x	An expression, character vector or filename with the odin code
type	An optional string indicating the the type of input - must be one of expression, file or text if provided. This skips the type detection code used by odin and makes validating user input easier.
options	odin options; see odin_options. The primary options that affect the parse stage are validate and pretty.

12 odin_validate

Details

odin_validate will always return a list with the same elements:

success A boolean, TRUE if validation was successful

result The intermediate representation, as returned by odin_parse_, if the validation was successful, otherwise NULL

error An error object if the validation was unsuccessful, otherwise NULL. This may be a classed odin error, in which case it will contain source location information - see the examples for details.

messages A list of messages, if the validation returned any. At present this is only non-fatal information about unused variables.

Author(s)

Rich FitzJohn

Examples

```
# A successful validation:
odin::odin_validate(c("deriv(x) <- 1", "initial(x) <- 1"))
# A complete failure:
odin::odin_validate("")
# A more interesting failure
code \leftarrow c("deriv(x) \leftarrow a", "initial(x) \leftarrow 1")
res <- odin::odin_validate(code)</pre>
# The object 'res$error' is an 'odin_error' object:
res$error
# It contains information that might be used to display to a
# user information about the error:
unclass(res$error)
# Notes are raised in a similar way:
code <- c("deriv(x) <- 1", "initial(x) <- 1", "a <- 1")
res <- odin::odin_validate(code)</pre>
res$messages[[1]]
```

Index

```
can\_compile, 2
coef, 6
odin, 3, 5
odin_ (odin), 3
odin_build, 5, 11
odin_ir, 4, 6
odin_ir_deserialise, 7
odin_options, 5, 7, 10, 11
odin_package, 4, 9
odin_parse, 5, 7, 10, 11
odin_parse_, 11, 12
\verb"odin_parse_" (\verb"odin_parse"), 10
odin_validate, 5, 7, 11, 11
pkgbuild::find_rtools(), 2
proc.time, 5
tempdir(), 3, 8
```