Package ‘odin’

October 2, 2023

Title ODE Generation and Integration

Version 1.2.5

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.

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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
can_compile

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

\[
\text{can_compile}(\text{verbose} = \text{FALSE}, \text{refresh} = \text{FALSE})
\]

Arguments

- `verbose`: Be verbose when running commands?
- `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 rtools installed. Using `pkgbuild::find_rtools()` with `debug = TRUE` may be helpful for diagnosing compiler issues.
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_checkUnused_equations = NULL, options = NULL)
```

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

**Arguments**

- `x` 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.
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 go-
ing), 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

```r
## 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
```
## 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).

```r
mod <- exp_decay$new()
```

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

---

**odin_build**

_Be the 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

```r
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.
# 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)

---

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)
```
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

x  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)

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.
odin_options(\texttt{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

\texttt{verbose} \hspace{1em} Logical scalar indicating if the compilation should be verbose. Defaults to the value of the option \texttt{odin.verbose} or \texttt{FALSE} otherwise.

\texttt{target} \hspace{1em} Compilation target. Options are "c" and "r", defaulting to the option \texttt{odin.target} or "c" otherwise.

\texttt{workdir} \hspace{1em} Directory to use for any generated files. This is only relevant for the "c" target. Defaults to the value of the option \texttt{odin.workdir} or \texttt{tempdir()} otherwise.

\texttt{validate} \hspace{1em} 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 \texttt{odin.validate} or \texttt{FALSE} otherwise.

\texttt{pretty} \hspace{1em} 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 \texttt{odin.pretty} or \texttt{FALSE} otherwise.

\texttt{skip_cache} \hspace{1em} 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 \texttt{odin.skip_cache} or \texttt{FALSE} otherwise.

\texttt{compiler_warnings} \hspace{1em} 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 \texttt{pkgbuild}.

\texttt{no_check_unused_equations} \hspace{1em} If \texttt{TRUE}, then don’t print messages about unused variables. Defaults to the option \texttt{odin.no_check_unused_equations} or \texttt{FALSE} otherwise.

\texttt{rewrite_dims} \hspace{1em} Logical, indicating if odin should try and rewrite your model dimensions (if using arrays). If \texttt{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 \texttt{TRUE} because parts of the model have been effectively evaluated during processing.

\texttt{rewrite_constants} \hspace{1em} Logical, indicating if odin should try and rewrite \textit{all} constant scalars. This is a superset of \texttt{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.
### 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

```r
odin_options()
```

---

### odin_package

*Create odin model in a package*

#### Description

Create an odin model within an existing package.

#### Usage

```r
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")` 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.
Examples

```r
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"))
```

---

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

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

odin_parse_(x, options = NULL, type = 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.

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

_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

```r
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.

### Examples

```r
# 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)
```
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

```r
# A successful validation:
odin::odin_validate(c("deriv(x) <- 1", "initial(x) <- 1"))

# A complete failure:
odin::odin_validate(""

# A more interesting failure
code <- c("deriv(x) <- a", "initial(x) <- 1")
res <- odin::odin_validate(code)
res

# 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)
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
odin_parse_(odin_parse), 10
odin_validate, 5, 7, 11, 11

pkgbuild::find_rtools(), 2
proc.time, 5

tempdir(), 3, 8