

# Package ‘rODE’

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**Type** Package

**Title** Ordinary Differential Equation (ODE) Solvers Written in R Using S4 Classes

**Version** 0.99.6

**Description** Show physics, math and engineering students how an ODE solver is made and how effective R classes can be for the construction of the equations that describe natural phenomena. Inspiration for this work comes from the book on ``Computer Simulations in Physics" by Harvey Gould, Jan Tobochnik, and Wolfgang Christian.

Book link: <<http://www.compadre.org/osp/items/detail.cfm?ID=7375>>.

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 rODE-package

*Ordinary Differential Equations*


---

### Description

Ordinary Differential Equations rODE.

---

AbstractODESolver-class

*AbstractODESolver class*

---

### Description

Defines the basic methods for all the ODE solvers.

AbstractODESolver generic

AbstractODESolver constructor missing

AbstractODESolver constructor ODE. Uses this constructor when ODE object is passed

### Usage

```
AbstractODESolver(ode, ...)
```

```
## S4 method for signature 'AbstractODESolver'  
step(object, ...)
```

```
## S4 method for signature 'AbstractODESolver'  
getODE(object, ...)
```

```
## S4 method for signature 'AbstractODESolver'  
setStepSize(object, stepSize, ...)
```

```
## S4 method for signature 'AbstractODESolver'  
init(object, stepSize, ...)
```

```
## S4 replacement method for signature 'AbstractODESolver'  
init(object, ...) <- value
```

```
## S4 method for signature 'AbstractODESolver'  
getStepSize(object, ...)
```

```
## S4 method for signature 'missing'  
AbstractODESolver(ode, ...)
```

```
## S4 method for signature 'ODE'  
AbstractODESolver(ode, ...)
```

### Arguments

ode	an ODE object
...	additional parameters
object	a class object
stepSize	the size of the step
value	the step size value

**Details**

Inherits from: ODESolver class

**Examples**

```
# This is how we start defining a new ODE solver: Euler
.Euler <- setClass("Euler",          # Euler solver very simple; no slots
  contains = c("AbstractODESolver"))

# Here we define the ODE solver Verlet
.Verlet <- setClass("Verlet", slots = c(
  rate1 = "numeric",                # Verlet calculates two rates
  rate2 = "numeric",
  rateCounter = "numeric"),
  contains = c("AbstractODESolver"))

# This is the definition of the ODE solver Runge-Kutta 4
.RK4 <- setClass("RK4", slots = c(   # On the other hand RK4 uses 4 rates
  rate1 = "numeric",
  rate2 = "numeric",
  rate3 = "numeric",
  rate4 = "numeric",
  estimated_state = "numeric"),     # and estimates another state
  contains = c("AbstractODESolver"))
```

---

DormandPrince45-class *DormandPrince45 ODE solver class*

---

**Description**

DormandPrince45 ODE solver class

DormandPrince45 generic

DormandPrince45 constructor ODE

**Usage**

```
DormandPrince45(ode, ...)
```

```
## S4 method for signature 'DormandPrince45'
init(object, stepSize, ...)
```

```
## S4 replacement method for signature 'DormandPrince45'
init(object, ...) <- value
```

```

## S4 method for signature 'DormandPrince45'
step(object, ...)

## S4 method for signature 'DormandPrince45'
enableRuntimeExceptions(object, enable)

## S4 method for signature 'DormandPrince45'
setStepSize(object, stepSize, ...)

## S4 method for signature 'DormandPrince45'
getStepSize(object, ...)

## S4 method for signature 'DormandPrince45'
setTolerance(object, tol)

## S4 replacement method for signature 'DormandPrince45'
setTolerance(object, ...) <- value

## S4 method for signature 'DormandPrince45'
getTolerance(object)

## S4 method for signature 'DormandPrince45'
getErrorCode(object)

## S4 method for signature 'ODE'
DormandPrince45(ode, ...)

```

### Arguments

ode	ODE object
...	additional parameters
object	a class object
stepSize	size of the step
value	step size to set
enable	a logical flag
tol	tolerance

### Examples

```

# ~~~~~ base class: KeplerVerlet.R

setClass("KeplerDormandPrince45", slots = c(
  GM = "numeric",
  odeSolver = "DormandPrince45",
  counter = "numeric"
),
contains = c("ODE")

```

```

)

setMethod("initialize", "KeplerDormandPrince45", function(.Object, ...) {
  .Object@GM <- 4 * pi * pi      # gravitation constant times combined mass
  .Object@state <- vector("numeric", 5) # x, vx, y, vy, t
  .Object@odeSolver <- DormandPrince45(.Object)
  .Object@counter <- 0
  return(.Object)
})

setMethod("doStep", "KeplerDormandPrince45", function(object, ...) {
  object@odeSolver <- step(object@odeSolver)
  object@state <- object@odeSolver@ode@state
  object
})

setMethod("getTime", "KeplerDormandPrince45", function(object, ...) {
  return(object@state[5])
})

setMethod("getEnergy", "KeplerDormandPrince45", function(object, ...) {
  ke <- 0.5 * (object@state[2] * object@state[2] +
              object@state[4] * object@state[4])
  pe <- -object@GM / sqrt(object@state[1] * object@state[1] +
                          object@state[3] * object@state[3])
  return(pe+ke)
})

setMethod("init", "KeplerDormandPrince45", function(object, initState, ...) {
  object@state <- initState
  # call init in AbstractODESolver
  object@odeSolver <- init(object@odeSolver, getStepSize(object@odeSolver))
  object@counter <- 0
  object
})

setReplaceMethod("init", "KeplerDormandPrince45", function(object, ..., value) {
  object@state <- value
  # call init in AbstractODESolver
  object@odeSolver <- init(object@odeSolver, getStepSize(object@odeSolver))
  object@counter <- 0
  object
})

setMethod("getRate", "KeplerDormandPrince45", function(object, state, ...) {
  # Computes the rate using the given state.
  r2 <- state[1] * state[1] + state[3] * state[3] # distance squared
  r3 <- r2 * sqrt(r2) # distance cubed
  object@rate[1] <- state[2]
  object@rate[2] <- (- object@GM * state[1]) / r3
  object@rate[3] <- state[4]
  object@rate[4] <- (- object@GM * state[3]) / r3
  object@rate[5] <- 1 # time derivative
})

```



```

        rate.counts = getRateCounts(ode),
        time = time )
    ode_solver <- step(ode_solver)      # advance solver one step
    stepSize <- getStepSize(ode_solver) # get the current step size
    time <- time + stepSize
    ode <- getODE(ode_solver)          # get updated ODE object
    state <- getState(ode)             # get the `state` vector
    i <- i + 1                          # add a row vector
  }
  DT <- data.table::rbindlist(rowVector) # create data table
  return(DT)
}

solution <- ComparisonRK45ODEApp()
plot(solution)

# additional plot for analytics solution vs. RK45 solver
solution.multi <- solution %>%
  select(t, ODE, exact)
plot(solution.multi)          # 3x3 plot

# plot comparative curves analytical vs ODE solver
solution.2x1 <- solution.multi %>%
  gather(key, value, -t)      # make a table of 3 variables. key: ODE/exact

g <- ggplot(solution.2x1, mapping = aes(x = t, y = value, color = key))
g <- g + geom_line(size = 1) +
  labs(title = "ODE vs Exact solution",
        subtitle = "tolerance = 1E-6")
print(g)

```

---

doStep

*doStep*


---

### Description

Perform a step

### Usage

```
doStep(object, ...)
```

### Arguments

object	a class object
...	additional parameters

**Examples**

```

# ++++++ example: PlanetApp.R
# Simulation of Earth orbiting around the Sun using the Euler ODE solver

importFromExamples("Planet.R")      # source the class

PlanetApp <- function(verbose = FALSE) {
  # x = 1, AU or Astronomical Units. Length of semimajor axis or the orbit
  # of the Earth around the Sun.
  x <- 1; vx <- 0; y <- 0; vy <- 6.28; t <- 0
  state <- c(x, vx, y, vy, t)
  dt <- 0.01
  planet <- Planet()
  planet@odeSolver <- setStepSize(planet@odeSolver, dt)
  planet <- init(planet, initState = state)
  rowvec <- vector("list")
  i <- 1
  # run infinite loop. stop with ESCAPE.
  while (getState(planet)[5] <= 90) {      # Earth orbit is 365 days around the sun
    rowvec[[i]] <- list(t = getState(planet)[5],      # just doing 3 months
                       x = getState(planet)[1],      # to speed up for CRAN
                       vx = getState(planet)[2],
                       y = getState(planet)[3],
                       vy = getState(planet)[4])
    for (j in 1:5) {                          # advances time
      planet <- doStep(planet)
    }
    i <- i + 1
  }
  DT <- data.table::rbindlist(rowvec)
  return(DT)
}
# run the application
solution <- PlanetApp()
select_rows <- seq(1, nrow(solution), 10)      # do not overplot
solution <- solution[select_rows,]
plot(solution)

# ++++++ application: Logistic.R
# Simulates the logistic equation
importFromExamples("Logistic.R")

# Run the application
LogisticApp <- function(verbose = FALSE) {
  x <- 0.1
  vx <- 0
  r <- 2      # Malthusian parameter (rate of maximum population growth)
  K <- 10.0   # carrying capacity of the environment
  dt <- 0.01; tol <- 1e-3; tmax <- 10

  population <- Logistic()                    # create a Logistic ODE object

```

```

# Two ways of initializing the object
# population <- init(population, c(x, vx, 0), r, K)
init(population) <- list(initState = c(x, vx, 0),
                        r = r,
                        K = K)

odeSolver <- Verlet(population)      # select the solver

# Two ways of initializing the solver
# odeSolver <- init(odeSolver, dt)
init(odeSolver) <- dt

population@odeSolver <- odeSolver
# setSolver(population) <- odeSolver

rowVector <- vector("list")
i <- 1
while (getTime(population) <= tmax) {
  rowVector[[i]] <- list(t = getTime(population),
                        s1 = getState(population)[1],
                        s2 = getState(population)[2])
  population <- doStep(population)
  i <- i + 1
}
DT <- data.table::rbindlist(rowVector)
return(DT)
}
# show solution
solution <- LogisticApp()
plot(solution)

```

---

enableRuntimeExceptions

*enableRuntimeExceptions*

---

## Description

Enable Runtime Exceptions

## Usage

```
enableRuntimeExceptions(object, enable, ...)
```

## Arguments

object	a class object
enable	a boolean to enable exceptions
...	additional parameters

**Examples**

```
setMethod("enableRuntimeExceptions", "DormandPrince45", function(object, enable) {
  object@enableExceptions <- enable
})
```

---

Euler-class	<i>Euler ODE solver class</i>
-------------	-------------------------------

---

**Description**

Euler ODE solver class

Euler generic

Euler constructor when 'ODE' passed

Euler constructor 'missing' is passed

**Usage**

```
Euler(ode, ...)
```

```
## S4 method for signature 'Euler'
init(object, stepSize, ...)
```

```
## S4 method for signature 'Euler'
step(object, ...)
```

```
## S4 method for signature 'Euler'
setStepSize(object, stepSize, ...)
```

```
## S4 method for signature 'Euler'
getStepSize(object, ...)
```

```
## S4 method for signature 'ODE'
Euler(ode, ...)
```

```
## S4 method for signature 'missing'
Euler(ode, ...)
```

**Arguments**

ode	an ODE object
...	additional parameters
object	an internal object of the class
stepSize	the size of the step

**Examples**

```

# ++++++ application: RigidBodyNXFApp.R
# example of a nonstiff system is the system of equations describing
# the motion of a rigid body without external forces.

importFromExamples("RigidBody.R")

# run the application
RigidBodyNXFApp <- function(verbose = FALSE) {
  # load the R class that sets up the solver for this application
  y1 <- 0 # initial y1 value
  y2 <- 1 # initial y2 value
  y3 <- 1 # initial y3 value
  dt <- 0.01 # delta time for step

  body <- RigidBodyNXF(y1, y2, y3)
  solver <- Euler(body)
  solver <- setStepSize(solver, dt)
  rowVector <- vector("list")
  i <- 1
  # stop loop when the body hits the ground
  while (getState(body)[4] <= 12) {
    rowVector[[i]] <- list(t = getState(body)[4],
                          y1 = getState(body)[1],
                          y2 = getState(body)[2],
                          y3 = getState(body)[3])

    solver <- step(solver)
    body <- getODE(solver)
    i <- i + 1
  }
  DT <- data.table::rbindlist(rowVector)
  return(DT)
}

# get the data table from the app
solution <- RigidBodyNXFApp()
plot(solution)

# ++++++ example: FallingParticleApp.R
# Application that simulates the free fall of a ball using Euler ODE solver

importFromExamples("FallingParticleODE.R") # source the class

FallingParticleODEApp <- function(verbose = FALSE) {
  # initial values
  initial_y <- 10
  initial_v <- 0
  dt <- 0.01
  ball <- FallingParticleODE(initial_y, initial_v)
  solver <- Euler(ball) # set the ODE solver
  solver <- setStepSize(solver, dt) # set the step
  rowVector <- vector("list")

```

```

    i <- 1
    # stop loop when the ball hits the ground, state[1] is the vertical position
    while (getState(ball)[1] > 0) {
      rowVector[[i]] <- list(t = getState(ball)[3],
                            y = getState(ball)[1],
                            vy = getState(ball)[2])
      solver <- step(solver) # move one step at a time
      ball <- getODE(solver) # update the ball state
      i <- i + 1
    }
    DT <- data.table::rbindlist(rowVector)
    return(DT)
  }
# show solution
solution <- FallingParticleODEApp()
plot(solution)
# KeplerVerlet.R

setClass("Kepler", slots = c(
  GM = "numeric",
  odeSolver = "Euler",
  counter = "numeric"
),
  contains = c("ODE")
)

setMethod("initialize", "Kepler", function(.Object, ...) {
  .Object@GM <- 4 * pi * pi # gravitation constant times combined mass
  .Object@state <- vector("numeric", 5) # x, vx, y, vy, t
  .Object@odeSolver <- Euler(.Object)
  .Object@counter <- 0
  return(.Object)
})

setMethod("doStep", "Kepler", function(object, ...) {
  # cat("state@doStep=", object@state, "\n")
  object@odeSolver <- step(object@odeSolver)

  object@state <- object@odeSolver@ode@state

  # object@rate <- object@odeSolver@ode@rate
  # cat("\t", object@odeSolver@ode@state)
  object
})

setMethod("getTime", "Kepler", function(object, ...) {
  return(object@state[5])
})

setMethod("getEnergy", "Kepler", function(object, ...) {
  ke <- 0.5 * (object@state[2] * object@state[2] +

```

```

        object@state[4] * object@state[4])
    pe <- -object@GM / sqrt(object@state[1] * object@state[1] +
        object@state[3] * object@state[3])
    return(pe+ke)
  })

setMethod("init", "Kepler", function(object, initState, ...) {
  object@state <- initState
  object@odeSolver <- init(object@odeSolver, getStepSize(object@odeSolver))
  object@counter <- 0
  object
})

setReplaceMethod("init", "Kepler", function(object, ..., value) {
  object@state <- value
  object@odeSolver <- init(object@odeSolver, getStepSize(object@odeSolver))
  object@counter <- 0
  object
})

setMethod("getRate", "Kepler", function(object, state, ...) {
  # Computes the rate using the given state.
  r2 <- state[1] * state[1] + state[3] * state[3] # distance squared
  r3 <- r2 * sqrt(r2) # distance cubed
  object@rate[1] <- state[2]
  object@rate[2] <- (- object@GM * state[1]) / r3
  object@rate[3] <- state[4]
  object@rate[4] <- (- object@GM * state[3]) / r3
  object@rate[5] <- 1 # time derivative

  # object@state <- object@odeSolver@ode@state <- state
  # object@state <- state
  object@counter <- object@counter + 1
  object@rate
})

setMethod("getState", "Kepler", function(object, ...) {
  # Gets the state variables.
  return(object@state)
})

# constructor
Kepler <- function() {
  kepler <- new("Kepler")
  return(kepler)
}
# ++++++ example: PlanetApp.R
# Simulation of Earth orbiting around the Sun using the Euler ODE solver

importFromExamples("Planet.R") # source the class

```

```

PlanetApp <- function(verbose = FALSE) {
  # x = 1, AU or Astronomical Units. Length of semimajor axis or the orbit
  # of the Earth around the Sun.
  x <- 1; vx <- 0; y <- 0; vy <- 6.28; t <- 0
  state <- c(x, vx, y, vy, t)
  dt <- 0.01
  planet <- Planet()
  planet@odeSolver <- setStepSize(planet@odeSolver, dt)
  planet <- init(planet, initState = state)
  rowvec <- vector("list")
  i <- 1
  # run infinite loop. stop with ESCAPE.
  while (getState(planet)[5] <= 90) { # Earth orbit is 365 days around the sun
    rowvec[[i]] <- list(t = getState(planet)[5], # just doing 3 months
                       x = getState(planet)[1], # to speed up for CRAN
                       vx = getState(planet)[2],
                       y = getState(planet)[3],
                       vy = getState(planet)[4])
    for (j in 1:5) { # advances time
      planet <- doStep(planet)
    }
    i <- i + 1
  }
  DT <- data.table::rbindlist(rowvec)
  return(DT)
}
# run the application
solution <- PlanetApp()
select_rows <- seq(1, nrow(solution), 10) # do not overplot
solution <- solution[select_rows,]
plot(solution)

# ++++++ application: RigidBodyNXFApp.R
# example of a nonstiff system is the system of equations describing
# the motion of a rigid body without external forces.

importFromExamples("RigidBody.R")

# run the application
RigidBodyNXFApp <- function(verbose = FALSE) {
  # load the R class that sets up the solver for this application
  y1 <- 0 # initial y1 value
  y2 <- 1 # initial y2 value
  y3 <- 1 # initial y3 value
  dt <- 0.01 # delta time for step

  body <- RigidBodyNXF(y1, y2, y3)
  solver <- Euler(body)
  solver <- setStepSize(solver, dt)
  rowVector <- vector("list")
  i <- 1
  # stop loop when the body hits the ground
  while (getState(body)[4] <= 12) {

```

```

        rowVector[[i]] <- list(t = getState(body)[4],
                              y1 = getState(body)[1],
                              y2 = getState(body)[2],
                              y3 = getState(body)[3])
        solver <- step(solver)
        body <- getODE(solver)
        i <- i + 1
    }
    DT <- data.table::rbindlist(rowVector)
    return(DT)
}

# get the data table from the app
solution <- RigidBodyNXFApp()
plot(solution)

```

---

EulerRichardson-class *EulerRichardson ODE solver class*

---

### Description

EulerRichardson ODE solver class

EulerRichardson generic

EulerRichardson constructor ODE

### Usage

```

EulerRichardson(ode, ...)

## S4 method for signature 'EulerRichardson'
init(object, stepSize, ...)

## S4 method for signature 'EulerRichardson'
step(object, ...)

## S4 method for signature 'ODE'
EulerRichardson(ode, ...)

```

### Arguments

ode	an ODE object
...	additional parameters
object	internal passing object
stepSize	the size of the step

**Examples**

```

# ++++++ example: PendulumApp.R
# Simulation of a pendulum using the EulerRichardson ODE solver

suppressPackageStartupMessages(library(ggplot2))

importFromExamples("Pendulum.R") # source the class

PendulumApp <- function(verbose = FALSE) {
  # initial values
  theta <- 0.2
  thetaDot <- 0
  dt <- 0.1
  pendulum <- Pendulum()
  # pendulum@state[3] <- 0 # set time to zero, t = 0
  pendulum <- setState(pendulum, theta, thetaDot)
  pendulum <- setStepSize(pendulum, dt = dt) # using stepSize in RK4
  pendulum@odeSolver <- setStepSize(pendulum@odeSolver, dt) # set new step size
  rowvec <- vector("list")
  i <- 1
  while (getState(pendulum)[3] <= 40) {
    rowvec[[i]] <- list(t = getState(pendulum)[3], # time
                      theta = getState(pendulum)[1], # angle
                      thetadot = getState(pendulum)[2]) # derivative of angle
    pendulum <- step(pendulum)
    i <- i + 1
  }
  DT <- data.table::rbindlist(rowvec)
  return(DT)
}
# show solution
solution <- PendulumApp()
plot(solution)

```

---

getEnergy

*getEnergy*


---

**Description**

Get the calculated energy level

**Usage**

```
getEnergy(object, ...)
```

**Arguments**

object	a class object
...	additional parameters

**Examples**

```

# KeplerEnergy.R
#

setClass("KeplerEnergy", slots = c(
  GM      = "numeric",
  odeSolver = "Verlet",
  counter  = "numeric"
),
  contains = c("ODE")
)

setMethod("initialize", "KeplerEnergy", function(.Object, ...) {
  .Object@GM <- 4 * pi * pi      # gravitation constant times combined mass
  .Object@state <- vector("numeric", 5) # x, vx, y, vy, t
  # .Object@odeSolver <- Verlet(ode = .Object)
  .Object@odeSolver <- Verlet(.Object)
  .Object@counter <- 0
  return(.Object)
})

setMethod("doStep", "KeplerEnergy", function(object, ...) {
  object@odeSolver <- step(object@odeSolver)
  object@state <- object@odeSolver@ode@state
  object
})

setMethod("getTime", "KeplerEnergy", function(object, ...) {
  return(object@state[5])
})

setMethod("getEnergy", "KeplerEnergy", function(object, ...) {
  ke <- 0.5 * (object@state[2] * object@state[2] +
    object@state[4] * object@state[4])
  pe <- -object@GM / sqrt(object@state[1] * object@state[1] +
    object@state[3] * object@state[3])
  return(pe+ke)
})

setMethod("init", "KeplerEnergy", function(object, initState, ...) {
  object@state <- initState
  object@odeSolver <- init(object@odeSolver, getStepSize(object@odeSolver))
  object@counter <- 0
  object
})

setReplaceMethod("init", "KeplerEnergy", function(object, ..., value) {
  initState <- value
  object@state <- initState
  object@odeSolver <- init(object@odeSolver, getStepSize(object@odeSolver))
})

```

```

    object@counter <- 0
    object
  })

  setMethod("getRate", "KeplerEnergy", function(object, state, ...) {
    # Computes the rate using the given state.
    r2 <- state[1] * state[1] + state[3] * state[3] # distance squared
    r3 <- r2 * sqrt(r2) # distance cubed
    object@rate[1] <- state[2]
    object@rate[2] <- (- object@GM * state[1]) / r3
    object@rate[3] <- state[4]
    object@rate[4] <- (- object@GM * state[3]) / r3
    object@rate[5] <- 1 # time derivative

    object@counter <- object@counter + 1
    object@rate

  })

  setMethod("getState", "KeplerEnergy", function(object, ...) {
    # Gets the state variables.
    return(object@state)
  })

  # constructor
  KeplerEnergy <- function() {
    kepler <- new("KeplerEnergy")
    return(kepler)
  }

```

---

getErrorCode

*getErrorCode*


---

### Description

Get an error code

### Usage

```
getErrorCode(object, tol, ...)
```

### Arguments

object	a class object
tol	tolerance
...	additional parameters

**Examples**

```
setMethod("getErrorCode", "DormandPrince45", function(object) {
  return(object@error_code)
})
```

---

```
getExactSolution      getExactSolution
```

---

**Description**

Compare analytical and calculated solutions

**Usage**

```
getExactSolution(object, t, ...)
```

**Arguments**

object	a class object
t	time at which we are performing the evaluation
...	additional parameters

**Examples**

```
# ++++++ example: ComparisonRK45App.R
# Compares the solution by the RK45 ODE solver versus the analytical solution
# Example file: ComparisonRK45App.R
# ODE Solver: Runge-Kutta 45
# ODE class : RK45
# Base class: ODETest

importFromExamples("ODETest.R")

ComparisonRK45App <- function(verbose = FALSE) {
  ode <- new("ODETest")           # create an `ODETest` object
  ode_solver <- RK45(ode)         # select the ODE solver
  ode_solver <- setStepSize(ode_solver, 1) # set the step

  # Two ways of setting the tolerance
  # ode_solver <- setTolerance(ode_solver, 1e-8) # set the tolerance
  setTolerance(ode_solver) <- 1e-8

  time <- 0
  rowVector <- vector("list")
  i <- 1
  while (time < 50) {
    rowVector[[i]] <- list(t = getState(ode)[2],
                          s1 = getState(ode)[1],
```

```

        s2 = getState(ode)[2],
        xs = getExactSolution(ode, time),
        counts = getRateCounts(ode),
        time = time
    )
    ode_solver <- step(ode_solver)      # advance one step
    stepSize <- getStepSize(ode_solver)
    time <- time + stepSize
    ode <- getODE(ode_solver)          # get updated ODE object
    i <- i + 1
}
return(data.table::rbindlist(rowVector)) # a data table with the results
}
# show solution
solution <- ComparisonRK45App()      # run the example
plot(solution)
# ODETest.R
# Called as base class for examples:
#           ComparisonRK45App.R
#           ComparisonRK45ODEApp.R

#' ODETest as an example of ODE class inheritance
#'
#' ODETest is a base class for examples ComparisonRK45App.R and
#' ComparisonRK45ODEApp.R. ODETest also uses an environment variable to store
#' the rate counts.
#'
#' @rdname ODE-class-example
#' @include ODE.R
setClass("ODETest", slots = c(
  n      = "numeric",      # counts the number of getRate evaluations
  stack = "environment"   # environment object to accumulate rate counts
),
  contains = c("ODE")
)

setMethod("initialize", "ODETest", function(.Object, ...) {
  .Object@stack$rateCounts <- 0      # counter for rate calculations
  .Object@state <- c(5.0, 0.0)
  return(.Object)
})

#' @rdname getExactSolution-method
setMethod("getExactSolution", "ODETest", function(object, t, ...) {
  return(5.0 * exp(-t))
})

#' @rdname getState-method
setMethod("getState", "ODETest", function(object, ...) {
  object@state
})

#' @rdname getRate-method

```

```

setMethod("getRate", "ODETest", function(object, state, ...) {
  object@rate[1] <- - state[1]
  object@rate[2] <- 1          # rate of change of time, dt/dt
  # accumulate how many times the rate has been called to calculate
  object@stack$rateCounts <- object@stack$rateCounts + 1
  object@state <- state
  object@rate
})

#' @rdname getRateCounts-method
setMethod("getRateCounts", "ODETest", function(object, ...) {
  # use environment stack to accumulate rate counts
  object@stack$rateCounts
})

# constructor
ODETest <- function() {
  odetest <- new("ODETest")
  odetest
}

```

---

getODE

*getODE*


---

### Description

Get the ODE status from the solver

### Usage

```
getODE(object, ...)
```

### Arguments

object	a class object
...	additional parameters

---

getRate

*getRate*


---

### Description

Get a new rate given a state

### Usage

```
getRate(object, state, ...)
```

**Arguments**

object	a class object
state	current state
...	additional parameters

**Examples**

```

# Kepler models Keplerian orbits of a mass moving under the influence of an
# inverse square force by implementing the ODE interface.
# Kepler.R
#

setClass("Kepler", slots = c(
  GM = "numeric"
),
  contains = c("ODE")
)

setMethod("initialize", "Kepler", function(.Object, ...) {
  .Object@GM <- 1.0 # gravitation constant times combined mass
  .Object@state <- vector("numeric", 5) # x, vx, y, vy, t
  return(.Object)
})

setMethod("getState", "Kepler", function(object, ...) {
  # Gets the state variables.
  return(object@state)
})

setMethod("getRate", "Kepler", function(object, state, ...) {
  # Computes the rate using the given state.
  r2 <- state[1] * state[1] + state[3] * state[3] # distance squared
  r3 <- r2 * sqrt(r2) # distance cubed
  object@rate[1] <- state[2]
  object@rate[2] <- (- object@GM * state[1]) / r3
  object@rate[3] <- state[4]
  object@rate[4] <- (- object@GM * state[3]) / r3
  object@rate[5] <- 1 # time derivative

  object@rate
})

# constructor
Kepler <- function(r, v) {
  kepler <- new("Kepler")
  kepler@state[1] = r[1]
  kepler@state[2] = v[1]
  kepler@state[3] = r[2]
  kepler@state[4] = v[2]
  kepler@state[5] = 0
}

```

```

    return(kepler)
}

```

---

<code>getRateCounter</code>	<i>getRateCounter</i>
-----------------------------	-----------------------

---

## Description

Get the rate counter

## Usage

```
getRateCounter(object, ...)
```

## Arguments

<code>object</code>	a class object
<code>...</code>	additional parameters

## Details

How many times the rate has changed with a step

## Examples

```

# ++++++ example: ComparisonRK45App.R
# Compares the solution by the RK45 ODE solver versus the analytical solution
# Example file: ComparisonRK45App.R
# ODE Solver: Runge-Kutta 45
# ODE class : RK45
# Base class: ODETest

importFromExamples("ODETest.R")

ComparisonRK45App <- function(verbose = FALSE) {
  ode <- new("ODETest")           # create an `ODETest` object
  ode_solver <- RK45(ode)         # select the ODE solver
  ode_solver <- setStepSize(ode_solver, 1) # set the step

  # Two ways of setting the tolerance
  # ode_solver <- setTolerance(ode_solver, 1e-8) # set the tolerance
  setTolerance(ode_solver) <- 1e-8

  time <- 0
  rowVector <- vector("list")
  i <- 1
  while (time < 50) {
    rowVector[[i]] <- list(t = getState(ode)[2],
                          s1 = getState(ode)[1],

```

```

        s2 = getState(ode)[2],
        xs = getExactSolution(ode, time),
        counts = getRateCounts(ode),
        time = time
    )
    ode_solver <- step(ode_solver)      # advance one step
    stepSize <- getStepSize(ode_solver)
    time <- time + stepSize
    ode <- getODE(ode_solver)          # get updated ODE object
    i <- i + 1
  }
  return(data.table::rbindlist(rowVector)) # a data table with the results
}
# show solution
solution <- ComparisonRK45App()      # run the example
plot(solution)

```

---

getRateCounts	<i>getRateCounts</i>
---------------	----------------------

---

**Description**

Get the number of times that the rate has been calculated

**Usage**

```
getRateCounts(object, ...)
```

**Arguments**

object	a class object
...	additional parameters

---

getState	<i>getState</i>
----------	-----------------

---

**Description**

Get current state of the system

**Usage**

```
getState(object, ...)
```

**Arguments**

object	a class object
...	additional parameters

**Examples**

```

# ++++++ application: VanderPolApp.R
# Solution of the Van der Pol equation
#
importFromExamples("VanderPol.R")

# run the application
VanderpolApp <- function(verbose = FALSE) {
  # set the orbit into a predefined state.
  y1 <- 2; y2 <- 0; dt <- 0.1;
  rigid_body <- VanderPol(y1, y2)
  solver <- RK45(rigid_body)
  rowVector <- vector("list")
  i <- 1
  while (getState(rigid_body)[3] <= 20) {
    rowVector[[i]] <- list(t = getState(rigid_body)[3],
                          y1 = getState(rigid_body)[1],
                          y2 = getState(rigid_body)[2])
    solver <- step(solver)
    rigid_body <- getODE(solver)
    i <- i + 1
  }
  DT <- data.table::rbindlist(rowVector)
  return(DT)
}

# show solution
solution <- VanderpolApp()
plot(solution)

# ++++++ application: SpringRK4App.R
# Simulation of a spring considering no friction

importFromExamples("SpringRK4.R")

# run application
SpringRK4App <- function(verbose = FALSE) {
  theta <- 0
  thetaDot <- -0.2
  tmax <- 22; dt <- 0.1
  spring <- SpringRK4()
  spring@state[3] <- 0 # set time to zero, t = 0
  spring <- setState(spring, theta, thetaDot)
  # spring <- setStepSize(spring, dt = dt) # using stepSize in RK4
  spring@odeSolver <- setStepSize(spring@odeSolver, dt) # set new step size
  rowvec <- vector("list")
  i <- 1
  while (getState(spring)[3] <= tmax) {
    rowvec[[i]] <- list(t = getState(spring)[3], # angle
                       y1 = getState(spring)[1], # derivative of the angle
                       y2 = getState(spring)[2]) # time
  }
}

```

```

        i <- i + 1
        spring <- step(spring)
    }
    DT <- data.table::rbindlist(rowvec)
    return(DT)
}

# show solution
solution <- SpringRK4App()
plot(solution)

```

---

getStepSize

*getStepSize*


---

### Description

Get the current value of the step size

### Usage

```
getStepSize(object, ...)
```

### Arguments

object	a class object
...	additional parameters

### Examples

```

# ++++++ Example: ComparisonRK45ODEApp.R
# Updates the ODE state instead of using the internal state in the ODE solver
# Also plots the solver solution versus the analytical solution at a
# tolerance of 1e-6
# Example file: ComparisonRK45ODEApp.R
# ODE Solver: Runge-Kutta 45
# ODE class : RK45
# Base class: ODETest

library(ggplot2)
library(dplyr)
library(tidyr)

importFromExamples("ODETest.R")

ComparisonRK45ODEApp <- function(verbose = FALSE) {
  ode <- new("ODETest") # new ODE instance
  ode_solver <- RK45(ode) # select ODE solver
  ode_solver <- setStepSize(ode_solver, 1) # set the step

  # two ways to set tolerance

```

```

    # ode_solver <- setTolerance(ode_solver, 1e-6)
    setTolerance(ode_solver) <- 1e-6

    time <- 0
    rowVector <- vector("list")          # row vector
    i <- 1    # counter
    while (time < 50) {
      # add solution objects to a row vector
      rowVector[[i]] <- list(t      = getState(ode)[2],
                            ODE    = getState(ode)[1],
                            s2     = getState(ode)[2],
                            exact  = getExactSolution(ode, time),
                            rate.counts = getRateCounts(ode),
                            time = time )

      ode_solver <- step(ode_solver)      # advance solver one step
      stepSize <- getStepSize(ode_solver) # get the current step size
      time <- time + stepSize
      ode <- getODE(ode_solver)           # get updated ODE object
      state <- getState(ode)              # get the `state` vector
      i <- i + 1                          # add a row vector
    }
    DT <- data.table::rbindlist(rowVector) # create data table
    return(DT)
  }

solution <- ComparisonRK45ODEApp()
plot(solution)

# additional plot for analytics solution vs. RK45 solver
solution.multi <- solution %>%
  select(t, ODE, exact)
plot(solution.multi)          # 3x3 plot

# plot comparative curves analytical vs ODE solver
solution.2x1 <- solution.multi %>%
  gather(key, value, -t)      # make a table of 3 variables. key: ODE/exact

g <- ggplot(solution.2x1, mapping = aes(x = t, y = value, color = key))
g <- g + geom_line(size = 1) +
  labs(title = "ODE vs Exact solution",
        subtitle = "tolerance = 1E-6")
print(g)

```

**Description**

Get the elapsed time

**Usage**

```
getTime(object, ...)
```

**Arguments**

object            a class object  
...                additional parameters

**Examples**

```
# ++++++ application: Logistic.R
# Simulates the logistic equation
importFromExamples("Logistic.R")

# Run the application
LogisticApp <- function(verbose = FALSE) {
  x <- 0.1
  vx <- 0
  r <- 2            # Malthusian parameter (rate of maximum population growth)
  K <- 10.0        # carrying capacity of the environment
  dt <- 0.01; tol <- 1e-3; tmax <- 10

  population <- Logistic()            # create a Logistic ODE object

  # Two ways of initializing the object
  # population <- init(population, c(x, vx, 0), r, K)
  init(population) <- list(initState = c(x, vx, 0),
                           r = r,
                           K = K)

  odeSolver <- Verlet(population)     # select the solver

  # Two ways of initializing the solver
  # odeSolver <- init(odeSolver, dt)
  init(odeSolver) <- dt

  population@odeSolver <- odeSolver
  # setSolver(population) <- odeSolver

  rowVector <- vector("list")
  i <- 1
  while (getTime(population) <= tmax) {
    rowVector[[i]] <- list(t = getTime(population),
                           s1 = getState(population)[1],
                           s2 = getState(population)[2])
    population <- doStep(population)
    i <- i + 1
  }
}
```

```

    }
    DT <- data.table::rbindlist(rowVector)
    return(DT)
  }
  # show solution
  solution <- LogisticApp()
  plot(solution)
  # KeplerEnergy.R
  #

setClass("KeplerEnergy", slots = c(
  GM      = "numeric",
  odeSolver = "Verlet",
  counter  = "numeric"
),
  contains = c("ODE")
)

setMethod("initialize", "KeplerEnergy", function(.Object, ...) {
  .Object@GM <- 4 * pi * pi      # gravitation constant times combined mass
  .Object@state <- vector("numeric", 5) # x, vx, y, vy, t
  # .Object@odeSolver <- Verlet(ode = .Object)
  .Object@odeSolver <- Verlet(.Object)
  .Object@counter <- 0
  return(.Object)
})

setMethod("doStep", "KeplerEnergy", function(object, ...) {
  object@odeSolver <- step(object@odeSolver)
  object@state <- object@odeSolver@ode@state
  object
})

setMethod("getTime", "KeplerEnergy", function(object, ...) {
  return(object@state[5])
})

setMethod("getEnergy", "KeplerEnergy", function(object, ...) {
  ke <- 0.5 * (object@state[2] * object@state[2] +
              object@state[4] * object@state[4])
  pe <- -object@GM / sqrt(object@state[1] * object@state[1] +
                          object@state[3] * object@state[3])
  return(pe+ke)
})

setMethod("init", "KeplerEnergy", function(object, initState, ...) {
  object@state <- initState
  object@odeSolver <- init(object@odeSolver, getStepSize(object@odeSolver))
  object@counter <- 0
  object
})

```

```

setReplaceMethod("init", "KeplerEnergy", function(object, ..., value) {
  initState <- value
  object@state <- initState
  object@odeSolver <- init(object@odeSolver, getStepSize(object@odeSolver))
  object@counter <- 0
  object
})

setMethod("getRate", "KeplerEnergy", function(object, state, ...) {
  # Computes the rate using the given state.
  r2 <- state[1] * state[1] + state[3] * state[3] # distance squared
  r3 <- r2 * sqrt(r2) # distance cubed
  object@rate[1] <- state[2]
  object@rate[2] <- (- object@GM * state[1]) / r3
  object@rate[3] <- state[4]
  object@rate[4] <- (- object@GM * state[3]) / r3
  object@rate[5] <- 1 # time derivative

  object@counter <- object@counter + 1
  object@rate
})

setMethod("getState", "KeplerEnergy", function(object, ...) {
  # Gets the state variables.
  return(object@state)
})

# constructor
KeplerEnergy <- function() {
  kepler <- new("KeplerEnergy")
  return(kepler)
}

```

---

getTolerance

*getTolerance*


---

### Description

Get the tolerance for the solver

### Usage

```
getTolerance(object, ...)
```

### Arguments

object	a class object
...	additional parameters

---

```
importFromExamples    importFromExamples
```

---

**Description**

Source the R script

**Usage**

```
importFromExamples(aClassFile, aFolder = "examples")
```

**Arguments**

aClassFile	a file containing one or more classes
aFolder	a folder where examples are located

---

```
init                init
```

---

**Description**

Set initial values before starting the ODE solver

Set initial values before starting the ODE solver

**Usage**

```
init(object, ...)
```

```
init(object, ...) <- value
```

**Arguments**

object	a class object
...	additional parameters
value	a value to set

**Details**

Sets the tolerance like this: solver <- init(solver, dt) Not all super classes require an init method.

Sets the tolerance like this: init(solver) <- dt

**Examples**

```

# init method in Kepler.R
setMethod("init", "Kepler", function(object, initState, ...) {
  object@state <- initState
  object@odeSolver <- init(object@odeSolver, getStepSize(object@odeSolver))
  object@counter <- 0
  object
})

# init method in LogisticApp.R
setMethod("init", "Logistic", function(object, initState, r, K, ...) {
  object@r <- r
  object@K <- K
  object@state <- initState
  object@odeSolver <- init(object@odeSolver, getStepSize(object@odeSolver))
  object@counter <- 0
  object
})

# init method in Planet.R
setMethod("init", "Planet", function(object, initState, ...) {
  object@state <- object@odeSolver@ode@state <- initState
  # initialize providing the step size
  object@odeSolver <- init(object@odeSolver, getStepSize(object@odeSolver))
  object@rate <- object@odeSolver@ode@rate
  object@state <- object@odeSolver@ode@state
  object
})

```

---

ODE-class

*ODE class*


---

**Description**

Defines an ODE object for any solver

ODE constructor

**Usage**

```
ODE()
```

```
## S4 method for signature 'ODE'
getState(object, ...)
```

```
## S4 method for signature 'ODE'
getRate(object, state, ...)
```

**Arguments**

object	a class object
...	additional parameters
state	current state

**Examples**

```
# ++++++ example: PendulumApp.R
# Simulation of a pendulum using the EulerRichardson ODE solver

suppressPackageStartupMessages(library(ggplot2))

importFromExamples("Pendulum.R") # source the class

PendulumApp <- function(verbose = FALSE) {
  # initial values
  theta <- 0.2
  thetaDot <- 0
  dt <- 0.1
  pendulum <- Pendulum()
  # pendulum@state[3] <- 0 # set time to zero, t = 0
  pendulum <- setState(pendulum, theta, thetaDot)
  pendulum <- setStepSize(pendulum, dt = dt) # using stepSize in RK4
  pendulum@odeSolver <- setStepSize(pendulum@odeSolver, dt) # set new step size
  rowvec <- vector("list")
  i <- 1
  while (getState(pendulum)[3] <= 40) {
    rowvec[[i]] <- list(t = getState(pendulum)[3], # time
                      theta = getState(pendulum)[1], # angle
                      thetadot = getState(pendulum)[2]) # derivative of angle
    pendulum <- step(pendulum)
    i <- i + 1
  }
  DT <- data.table::rbindlist(rowvec)
  return(DT)
}

# show solution
solution <- PendulumApp()
plot(solution)
# ++++++ example: PendulumEulerApp.R
# Pendulum simulation with the Euler ODE solver
# Notice how Euler is not applicable in this case as it diverges very quickly
# even when it is using a very small `delta t`?ODE

importFromExamples("PendulumEuler.R") # source the class

PendulumEulerApp <- function(verbose = FALSE) {
  # initial values
  theta <- 0.2
  thetaDot <- 0
  dt <- 0.01

```

```

    pendulum <- PendulumEuler()
    pendulum@state[3] <- 0 # set time to zero, t = 0
    pendulum <- setState(pendulum, theta, thetaDot)
    stepSize <- dt
    pendulum <- setStepSize(pendulum, stepSize)
    pendulum@odeSolver <- setStepSize(pendulum@odeSolver, dt) # set new step size
    rowvec <- vector("list")
    i <- 1
    while (getState(pendulum)[3] <= 50) {
      rowvec[[i]] <- list(t = getState(pendulum)[3],
                        theta = getState(pendulum)[1],
                        thetaDot = getState(pendulum)[2])
      pendulum <- step(pendulum)
      i <- i + 1
    }
    DT <- data.table::rbindlist(rowvec)
    return(DT)
  }

solution <- PendulumEulerApp()
plot(solution)
# ++++++ example KeplerApp.R
# KeplerApp solves an inverse-square law model (Kepler model) using an adaptive
# stepsize algorithm.
# Application showing two planet orbiting
# File in examples: KeplerApp.R

importFromExamples("Kepler.R") # source the class Kepler

KeplerApp <- function(verbose = FALSE) {

  # set the orbit into a predefined state.
  r <- c(2, 0) # orbit radius
  v <- c(0, 0.25) # velocity
  dt <- 0.1
  planet <- Kepler(r, v) # make up an ODE object
  solver <- RK45(planet)
  rowVector <- vector("list")
  i <- 1
  while (getState(planet)[5] <= 10) {
    rowVector[[i]] <- list(t = planet@state[5],
                          planet1.r = getState(planet)[1],
                          planet1.v = getState(planet)[2],
                          planet2.r = getState(planet)[3],
                          planet2.v = getState(planet)[4])

    solver <- step(solver)
    planet <- getODE(solver)
    i <- i + 1
  }
  DT <- data.table::rbindlist(rowVector)

  return(DT)
}

```

```

solution <- KeplerApp()
plot(solution)

# ~~~~~ base class: FallingParticleODE.R
# Class definition for application FallingParticleODEApp.R

setClass("FallingParticleODE", slots = c(
  g = "numeric"
),
  prototype = prototype(
    g = 9.8
  ),
  contains = c("ODE")
)

setMethod("initialize", "FallingParticleODE", function(.Object, ...) {
  .Object@state <- vector("numeric", 3)
  return(.Object)
})

setMethod("getState", "FallingParticleODE", function(object, ...) {
  # Gets the state variables.
  return(object@state)
})

setMethod("getRate", "FallingParticleODE", function(object, state, ...) {
  # Gets the rate of change using the argument's state variables.
  object@rate[1] <- state[2]
  object@rate[2] <- - object@g
  object@rate[3] <- 1

  object@rate
})

# constructor
FallingParticleODE <- function(y, v) {
  .FallingParticleODE <- new("FallingParticleODE")
  .FallingParticleODE@state[1] <- y
  .FallingParticleODE@state[2] <- v
  .FallingParticleODE@state[3] <- 0
  .FallingParticleODE
}

```

---

ODEAdaptiveSolver-class

*ODEAdaptiveSolver class*

---

**Description**

Base class to be inherited by adaptive solvers such as RK45

ODEAdaptiveSolver generic

ODEAdaptiveSolver constructor

**Usage**

```
ODEAdaptiveSolver(...)
```

```
## S4 method for signature 'ODEAdaptiveSolver'
setTolerance(object, tol)
```

```
## S4 replacement method for signature 'ODEAdaptiveSolver'
setTolerance(object, ...) <- value
```

```
## S4 method for signature 'ODEAdaptiveSolver'
getTolerance(object)
```

```
## S4 method for signature 'ODEAdaptiveSolver'
getErrorCode(object)
```

```
## S4 method for signature 'ANY'
ODEAdaptiveSolver(...)
```

**Arguments**

...	additional parameters
object	a class object
tol	tolerance
value	the value for the tolerance

---

ODESolver-class	<i>ODESolver virtual class</i>
-----------------	--------------------------------

---

**Description**

A virtual class inherited by AbstractODESolver

ODESolver constructor

Set initial values and get ready to start the solver

Set the size of the step

**Usage**

```
ODESolver(object, stepSize, ...)  
  
## S4 method for signature 'ODESolver'  
init(object, stepSize, ...)  
  
## S4 method for signature 'ODESolver'  
step(object, ...)  
  
## S4 method for signature 'ODESolver'  
getODE(object, ...)  
  
## S4 method for signature 'ODESolver'  
setStepSize(object, stepSize, ...)  
  
## S4 method for signature 'ODESolver'  
getStepSize(object, ...)
```

**Arguments**

object	a class object
stepSize	size of the step
...	additional parameters

**See Also**

Other ODESolver helpers: [ODESolverFactory-class](#)

---

ODESolverFactory-class

*ODESolverFactory*

---

**Description**

ODESolverFactory helps to create a solver given only the name as string

ODESolverFactory generic

This is a factory method that creates an ODESolver using a name.

ODESolverFactory constructor

**Usage**

```
ODESolverFactory(...)  
  
createODESolver(object, ...)
```

```
## S4 method for signature 'ODESolverFactory'
createODESolver(object, ode, solverName, ...)
```

```
## S4 method for signature 'ANY'
ODESolverFactory(...)
```

### Arguments

```
...           additional parameters
object        an solver object
ode           an ODE object
solverName    the desired solver as a string
```

### See Also

Other ODESolver helpers: [ODESolver-class](#)

Other ODESolver helpers: [ODESolver-class](#)

### Examples

```
# This example uses ODESolverFactory

importFromExamples("SHO.R")

# SHOApp.R
SHOApp <- function(...) {
  x <- 1.0; v <- 0; k <- 1.0; dt <- 0.01; tolerance <- 1e-3
  sho <- SHO(x, v, k)

  # Use ODESolverFactory
  solver_factory <- ODESolverFactory()
  solver <- createODESolver(solver_factory, sho, "DormandPrince45")
  # solver <- DormandPrince45(sho) # this can also be used

  # Two ways of setting the tolerance
  # solver <- setTolerance(solver, tolerance) # or this below
  setTolerance(solver) <- tolerance

  # Two ways of initializing the solver
  # solver <- init(solver, dt)
  init(solver) <- dt

  i <- 1; rowVector <- vector("list")
  while (getState(sho)[3] <= 500) {
    rowVector[[i]] <- list(x = getState(sho)[1],
                          v = getState(sho)[2],
                          t = getState(sho)[3])
    solver <- step(solver)
    sho <- getODE(solver)
    i <- i + 1
  }
}
```

```

    }
    return(data.table::rbindlist(rowVector))
}

solution <- SHOApp()
plot(solution)

# This example uses ODESolverFactory

importFromExamples("SHO.R")

# SHOApp.R
SHOApp <- function(...) {
  x <- 1.0; v <- 0; k <- 1.0; dt <- 0.01; tolerance <- 1e-3
  sho <- SHO(x, v, k)

  # Use ODESolverFactory
  solver_factory <- ODESolverFactory()
  solver <- createODESolver(solver_factory, sho, "DormandPrince45")
  # solver <- DormandPrince45(sho) # this can also be used

  # Two ways of setting the tolerance
  # solver <- setTolerance(solver, tolerance) # or this below
  setTolerance(solver) <- tolerance

  # Two ways of initializing the solver
  # solver <- init(solver, dt)
  init(solver) <- dt

  i <- 1; rowVector <- vector("list")
  while (getState(sho)[3] <= 500) {
    rowVector[[i]] <- list(x = getState(sho)[1],
                          v = getState(sho)[2],
                          t = getState(sho)[3])

    solver <- step(solver)
    sho <- getODE(solver)
    i <- i + 1
  }
  return(data.table::rbindlist(rowVector))
}

solution <- SHOApp()
plot(solution)

```

**Description**

RK4 class  
 RK4 generic  
 RK4 class constructor

**Usage**

```
RK4(ode, ...)

## S4 method for signature 'RK4'
init(object, stepSize, ...)

## S4 replacement method for signature 'RK4'
init(object, ...) <- value

## S4 method for signature 'RK4'
step(object, ...)

## S4 method for signature 'ODE'
RK4(ode, ...)
```

**Arguments**

ode	an ODE object
...	additional parameters
object	internal passing object
stepSize	the size of the step
value	value for the step

**Examples**

```
# ~~~~~ base class: Projectile.R
# Projectile class to be solved with Euler method

setClass("Projectile", slots = c(
  g = "numeric",
  odeSolver = "RK4"
),
  prototype = prototype(
    g = 9.8
  ),
  contains = c("ODE")
)

setMethod("initialize", "Projectile", function(.Object) {
  .Object@odeSolver <- RK4(.Object)
  return(.Object)
})
```

```

}))

setMethod("setStepSize", "Projectile", function(object, stepSize, ...) {
  # use explicit parameter declaration
  # setStepSize generic has two step parameters: stepSize and dt
  object@odeSolver <- setStepSize(object@odeSolver, stepSize)
  object
}))

setMethod("step", "Projectile", function(object) {
  object@odeSolver <- step(object@odeSolver)
  object@rate <- object@odeSolver@odeRate
  object@state <- object@odeSolver@odeState
  object
}))

setMethod("setState", signature("Projectile"), function(object, x, vx, y, vy, ...) {
  object@state[1] <- x
  object@state[2] <- vx
  object@state[3] <- y
  object@state[4] <- vy
  object@state[5] <- 0 # t + dt
  object@odeSolver@odeState <- object@state
  object
}))

setMethod("getState", "Projectile", function(object) {
  object@state
}))

setMethod("getRate", "Projectile", function(object, state, ...) {
  object@rate[1] <- state[2] # rate of change of x
  object@rate[2] <- 0 # rate of change of vx
  object@rate[3] <- state[4] # rate of change of y
  object@rate[4] <- - object@g # rate of change of vy
  object@rate[5] <- 1 # dt/dt = 1

  object@rate
}))

# constructor
Projectile <- function() new("Projectile")
# ++++++ example: PendulumApp.R
# Simulation of a pendulum using the EulerRichardson ODE solver

suppressPackageStartupMessages(library(ggplot2))

importFromExamples("Pendulum.R") # source the class

```

```

PendulumApp <- function(verbose = FALSE) {
  # initial values
  theta <- 0.2
  thetaDot <- 0
  dt <- 0.1
  pendulum <- Pendulum()
  # pendulum@state[3] <- 0      # set time to zero, t = 0
  pendulum <- setState(pendulum, theta, thetaDot)
  pendulum <- setStepSize(pendulum, dt = dt) # using stepSize in RK4
  pendulum@odeSolver <- setStepSize(pendulum@odeSolver, dt) # set new step size
  rowvec <- vector("list")
  i <- 1
  while (getState(pendulum)[3] <= 40) {
    rowvec[[i]] <- list(t      = getState(pendulum)[3], # time
                      theta  = getState(pendulum)[1], # angle
                      thetadot = getState(pendulum)[2]) # derivative of angle
    pendulum <- step(pendulum)
    i <- i + 1
  }
  DT <- data.table::rbindlist(rowvec)
  return(DT)
}

# show solution
solution <- PendulumApp()
plot(solution)
# ++++++ application: ReactionApp.R
# ReactionApp solves an autocatalytic oscillating chemical
# reaction (Brusselator model) using
# a fourth-order Runge-Kutta algorithm.

importFromExamples("Reaction.R") # source the class

ReactionApp <- function(verbose = FALSE) {
  X <- 1; Y <- 5;
  dt <- 0.1

  reaction <- Reaction(c(X, Y, 0))
  solver <- RK4(reaction)
  rowvec <- vector("list")
  i <- 1
  while (getState(reaction)[3] < 100) { # stop at t = 100
    rowvec[[i]] <- list(t = getState(reaction)[3],
                      X = getState(reaction)[1],
                      Y = getState(reaction)[2])
    solver <- step(solver)
    reaction <- getODE(solver)
    i <- i + 1
  }
  DT <- data.table::rbindlist(rowvec)
  return(DT)
}

```



```

        counts = getRateCounts(ode),
        time   = time
      )
      ode_solver <- step(ode_solver)      # advance one step
      stepSize  <- getStepSize(ode_solver)
      time <- time + stepSize
      ode <- getODE(ode_solver)          # get updated ODE object
      i <- i + 1
    }
    return(data.table::rbindlist(rowVector)) # a data table with the results
  }
# show solution
solution <- ComparisonRK45App()          # run the example
plot(solution)
# ++++++ example KeplerApp.R
# KeplerApp solves an inverse-square law model (Kepler model) using an adaptive
# stepsize algorithm.
# Application showing two planet orbiting
# File in examples: KeplerApp.R

importFromExamples("Kepler.R") # source the class Kepler

KeplerApp <- function(verbose = FALSE) {

  # set the orbit into a predefined state.
  r <- c(2, 0)                          # orbit radius
  v <- c(0, 0.25)                        # velocity
  dt <- 0.1
  planet <- Kepler(r, v)                 # make up an ODE object
  solver <- RK45(planet)
  rowVector <- vector("list")
  i <- 1
  while (getState(planet)[5] <= 10) {
    rowVector[[i]] <- list(t = planet@state[5],
                          planet1.r = getState(planet)[1],
                          planet1.v = getState(planet)[2],
                          planet2.r = getState(planet)[3],
                          planet2.v = getState(planet)[4])

    solver <- step(solver)
    planet <- getODE(solver)
    i <- i + 1
  }
  DT <- data.table::rbindlist(rowVector)

  return(DT)
}

solution <- KeplerApp()
plot(solution)

```

---

```
run_test_applications  run_test_applications
```

---

**Description**

Run test all the examples

**Usage**

```
run_test_applications()
```

---

```
setSolver<-           setSolver
```

---

**Description**

Set a solver over an ODE object

**Usage**

```
setSolver(object) <- value
```

**Arguments**

object	a class object
value	value to be set

---

```
setState              setState
```

---

**Description**

New setState that should work with different methods "theta", "thetaDot": used in PendulumApp  
"x", "vx", "y", "vy": used in ProjectileApp

**Usage**

```
setState(object, ...)
```

**Arguments**

object	a class object
...	additional parameters

**Examples**

```

# ++++++ application: ProjectileApp.R
#                                     test Projectile with RK4
#                                     originally uses Euler

# suppressMessages(library(data.table))

importFromExamples("Projectile.R")      # source the class

ProjectileApp <- function(verbose = FALSE) {
  # initial values
  x <- 0; vx <- 10; y <- 0; vy <- 10
  state <- c(x, vx, y, vy, 0)           # state vector
  dt <- 0.01

  projectile <- Projectile()
  projectile <- setState(projectile, x, vx, y, vy)

  projectile@odeSolver <- init(projectile@odeSolver, 0.123)

  # init(projectile) <- 0.123

  projectile@odeSolver <- setStepSize(projectile@odeSolver, dt)
  rowV <- vector("list")
  i <- 1
  while (getState(projectile)[3] >= 0) {
    rowV[[i]] <- list(t = getState(projectile)[5],
                     x = getState(projectile)[1],
                     vx = getState(projectile)[2],
                     y = getState(projectile)[3],      # vertical position
                     vy = getState(projectile)[4])
    projectile <- step(projectile)
    i <- i + 1
  }
  DT <- data.table::rbindlist(rowV)
  return(DT)
}

solution <- ProjectileApp()
plot(solution)
# ++++++ example: PendulumApp.R
# Simulation of a pendulum using the EulerRichardson ODE solver

suppressPackageStartupMessages(library(ggplot2))

importFromExamples("Pendulum.R")      # source the class

PendulumApp <- function(verbose = FALSE) {
  # initial values
  theta <- 0.2
  thetaDot <- 0

```

```

dt <- 0.1
pendulum <- Pendulum()
# pendulum@state[3] <- 0      # set time to zero, t = 0
pendulum <- setState(pendulum, theta, thetaDot)
pendulum <- setStepSize(pendulum, dt = dt) # using stepSize in RK4
pendulum@odeSolver <- setStepSize(pendulum@odeSolver, dt) # set new step size
rowvec <- vector("list")
i <- 1
while (getState(pendulum)[3] <= 40) {
  rowvec[[i]] <- list(t      = getState(pendulum)[3], # time
                    theta   = getState(pendulum)[1], # angle
                    thetadot = getState(pendulum)[2]) # derivative of angle
  pendulum <- step(pendulum)
  i <- i + 1
}
DT <- data.table::rbindlist(rowvec)
return(DT)
}
# show solution
solution <- PendulumApp()
plot(solution)

```

---

setStepSize

*setStepSize*


---

## Description

setStepSize uses either of two step parameters: stepSize and dt stepSize works for most of the applications dt is used in Pendulum

## Usage

```
setStepSize(object, ...)
```

## Arguments

object	a class object
...	additional parameters

## Examples

```

# ++++++application: SpringRK4App.R
# Simulation of a spring considering no friction

importFromExamples("SpringRK4.R")

# run application
SpringRK4App <- function(verbose = FALSE) {

```

```

theta    <- 0
thetaDot <- -0.2
tmax     <- 22; dt <- 0.1
spring <- SpringRK4()
spring@state[3] <- 0      # set time to zero, t = 0
spring <- setState(spring, theta, thetaDot)
# spring <- setStepSize(spring, dt = dt) # using stepSize in RK4
spring@odeSolver <- setStepSize(spring@odeSolver, dt) # set new step size
rowvec <- vector("list")
i <- 1
while (getState(spring)[3] <= tmax) {
  rowvec[[i]] <- list(t = getState(spring)[3],      # angle
                    y1 = getState(spring)[1],      # derivative of the angle
                    y2 = getState(spring)[2])      # time
  i <- i + 1
  spring <- step(spring)
}
DT <- data.table::rbindlist(rowvec)
return(DT)
}

# show solution
solution <- SpringRK4App()
plot(solution)
# ++++++ example: ComparisonRK45App.R
# Compares the solution by the RK45 ODE solver versus the analytical solution
# Example file: ComparisonRK45App.R
# ODE Solver: Runge-Kutta 45
# ODE class : RK45
# Base class: ODETest

importFromExamples("ODETest.R")

ComparisonRK45App <- function(verbose = FALSE) {
  ode <- new("ODETest")      # create an `ODETest` object
  ode_solver <- RK45(ode)    # select the ODE solver
  ode_solver <- setStepSize(ode_solver, 1)  # set the step

  # Two ways of setting the tolerance
  # ode_solver <- setTolerance(ode_solver, 1e-8) # set the tolerance
  setTolerance(ode_solver) <- 1e-8

  time <- 0
  rowVector <- vector("list")
  i <- 1
  while (time < 50) {
    rowVector[[i]] <- list(t = getState(ode)[2],
                          s1 = getState(ode)[1],
                          s2 = getState(ode)[2],
                          xs = getExactSolution(ode, time),
                          counts = getRateCounts(ode),
                          time = time
                          )
  }
}

```

```

        ode_solver <- step(ode_solver)           # advance one step
        stepSize  <- getStepSize(ode_solver)
        time <- time + stepSize
        ode <- getODE(ode_solver)               # get updated ODE object
        i <- i + 1
    }
    return(data.table::rbindlist(rowVector))    # a data table with the results
}
# show solution
solution <- ComparisonRK45App()               # run the example
plot(solution)

```

---

```

setTolerance      setTolerance

```

---

## Description

Set the tolerance for the solver

Set the tolerance for the solver

## Usage

```

setTolerance(object, tol)

setTolerance(object, ...) <- value

```

## Arguments

object	a class object
tol	tolerance
...	additional parameters
value	a value to set

## Details

Sets the tolerance like this: `odeSolver <- setTolerance(odeSolver, tol)`

Sets the tolerance like this: `setTolerance(odeSolver) <- tol`

## Examples

```

# ++++++ example: ComparisonRK45App.R
# Compares the solution by the RK45 ODE solver versus the analytical solution
# Example file: ComparisonRK45App.R
# ODE Solver:   Runge-Kutta 45
# ODE class :   RK45
# Base class:   ODETest

importFromExamples("ODETest.R")

```

```

ComparisonRK45App <- function(verbose = FALSE) {
  ode <- new("ODETest")           # create an `ODETest` object
  ode_solver <- RK45(ode)         # select the ODE solver
  ode_solver <- setStepSize(ode_solver, 1) # set the step

  # Two ways of setting the tolerance
  # ode_solver <- setTolerance(ode_solver, 1e-8) # set the tolerance
  setTolerance(ode_solver) <- 1e-8

  time <- 0
  rowVector <- vector("list")
  i <- 1
  while (time < 50) {
    rowVector[[i]] <- list(t = getState(ode)[2],
                          s1 = getState(ode)[1],
                          s2 = getState(ode)[2],
                          xs = getExactSolution(ode, time),
                          counts = getRateCounts(ode),
                          time = time
                          )
    ode_solver <- step(ode_solver) # advance one step
    stepSize <- getStepSize(ode_solver)
    time <- time + stepSize
    ode <- getODE(ode_solver)      # get updated ODE object
    i <- i + 1
  }
  return(data.table::rbindlist(rowVector)) # a data table with the results
}

# show solution
solution <- ComparisonRK45App() # run the example
plot(solution)
# ++++++ example: KeplerDormandPrince45App.R
# Demonstration of the use of ODE solver RK45 for a particle subjected to
# a inverse-law force. The difference with the example KeplerApp is we are
# seeing the effect in the x and y axis on the particle.
# The original routine used the Verlet ODE solver

importFromExamples("KeplerDormandPrince45.R")

set_solver <- function(ode_object, solver) {
  slot(ode_object, "odeSolver") <- solver
  ode_object
}

KeplerDormandPrince45App <- function(verbose = FALSE) {
  # values for the examples
  x <- 1
  vx <- 0
  y <- 0
  vy <- 2 * pi
  dt <- 0.01 # step size
  tol <- 1e-3 # tolerance
}

```

```

particle <- KeplerDormandPrince45() # use class Kepler

# Two ways of initializing the ODE object
# particle <- init(particle, c(x, vx, y, vy, 0)) # enter state vector
init(particle) <- c(x, vx, y, vy, 0)

odeSolver <- DormandPrince45(particle) # select the ODE solver

# Two ways of initializing the solver
# odeSolver <- init(odeSolver, dt) # start the solver
init(odeSolver) <- dt

# Two ways of setting the tolerance
# odeSolver <- setTolerance(odeSolver, tol) # this works for adaptive solvers
setTolerance(odeSolver) <- tol
setSolver(particle) <- odeSolver

initialEnergy <- getEnergy(particle) # calculate the energy
rowVector <- vector("list")
i <- 1
while (getTime(particle) < 1.5) {
  rowVector[[i]] <- list(t = getState(particle)[5],
                        x = getState(particle)[1],
                        vx = getState(particle)[2],
                        y = getState(particle)[3],
                        vx = getState(particle)[4],
                        energy = getEnergy(particle) )
  particle <- doStep(particle) # advance one step
  energy <- getEnergy(particle) # calculate energy
  i <- i + 1
}
DT <- data.table::rbindlist(rowVector)
return(DT)
}

solution <- KeplerDormandPrince45App()
plot(solution)

importFromExamples("AdaptiveStep.R")

# running function
AdaptiveStepApp <- function(verbose = FALSE) {
  ode <- new("Impulse")
  ode_solver <- RK45(ode)

  # Two ways to initialize the solver
  # ode_solver <- init(ode_solver, 0.1)
  init(ode_solver) <- 0.1

  # two ways to set tolerance
  # ode_solver <- setTolerance(ode_solver, 1.0e-4)
  setTolerance(ode_solver) <- 1.0e-4
}

```

```

    i <- 1; rowVector <- vector("list")
    while (getState(ode)[1] < 12) {
      rowVector[[i]] <- list(s1 = getState(ode)[1],
                           s2 = getState(ode)[2],
                           t  = getState(ode)[3])
      ode_solver <- step(ode_solver)
      ode <- getODE(ode_solver)
      i <- i + 1
    }
    return(data.table::rbindlist(rowVector))
  }

# run application
solution <- AdaptiveStepApp()
plot(solution)

```

---

showMethods2

*showMethods2*


---

### Description

Get the methods in a class. But only those specific to the class

### Usage

```
showMethods2(theClass)
```

### Arguments

theClass      class to analyze

---

step

*step*


---

### Description

Advances a step within the ODE solver

### Usage

```
step(object, ...)
```

### Arguments

object      a class object  
...          additional parameters

**Examples**

```

# ++++++ application: ReactionApp.R
# ReactionApp solves an autocatalytic oscillating chemical
# reaction (Brusselator model) using
# a fourth-order Runge-Kutta algorithm.

importFromExamples("Reaction.R")      # source the class

ReactionApp <- function(verbose = FALSE) {
  X <- 1; Y <- 5;
  dt <- 0.1

  reaction <- Reaction(c(X, Y, 0))
  solver <- RK4(reaction)
  rowvec <- vector("list")
  i <- 1
  while (getState(reaction)[3] < 100) {          # stop at t = 100
    rowvec[[i]] <- list(t = getState(reaction)[3],
                       X = getState(reaction)[1],
                       Y = getState(reaction)[2])
    solver <- step(solver)
    reaction <- getODE(solver)
    i <- i + 1
  }
  DT <- data.table::rbindlist(rowvec)
  return(DT)
}

solution <- ReactionApp()
plot(solution)

```

---

Verlet-class

*Verlet ODE solver class*


---

**Description**

Verlet ODE solver class

Verlet generic

Verlet class constructor ODE

**Usage**

Verlet(ode, ...)

```
## S4 method for signature 'Verlet'
init(object, stepSize, ...)
```

```
## S4 method for signature 'Verlet'
getRateCounter(object, ...)

## S4 method for signature 'Verlet'
step(object, ...)

## S4 method for signature 'ODE'
Verlet(ode, ...)
```

### Arguments

ode	an ODE object
...	additional parameters
object	a class object
stepSize	size of the step

### Examples

```
# ++++++ example: KeplerEnergyApp.R
# Demonstration of the use of the Verlet ODE solver
#

importFromExamples("KeplerEnergy.R") # source the class Kepler

KeplerEnergyApp <- function(verbose = FALSE) {
  # initial values
  x <- 1
  vx <- 0
  y <- 0
  vy <- 2 * pi
  dt <- 0.01
  tol <- 1e-3
  particle <- KeplerEnergy()

  # Two ways of initializing the ODE object
  # particle <- init(particle, c(x, vx, y, vy, 0))
  init(particle) <- c(x, vx, y, vy, 0)

  odeSolver <- Verlet(particle)

  # Two ways of initializing the solver
  # odeSolver <- init(odeSolver, dt)
  init(odeSolver) <- dt

  particle@odeSolver <- odeSolver
  initialEnergy <- getEnergy(particle)
  rowVector <- vector("list")
  i <- 1
  while (getTime(particle) <= 1.20) {
    rowVector[[i]] <- list(t = getState(particle)[5],
```

```

        x = getState(particle)[1],
        vx = getState(particle)[2],
        y = getState(particle)[3],
        vy = getState(particle)[4],
        E = getEnergy(particle)
    particle <- doStep(particle)
    energy <- getEnergy(particle)
    i <- i + 1
  }
  DT <- data.table::rbindlist(rowVector)
  return(DT)
}

solution <- KeplerEnergyApp()
plot(solution)

# ++++++ application: Logistic.R
# Simulates the logistic equation
importFromExamples("Logistic.R")

# Run the application
LogisticApp <- function(verbose = FALSE) {
  x <- 0.1
  vx <- 0
  r <- 2      # Malthusian parameter (rate of maximum population growth)
  K <- 10.0   # carrying capacity of the environment
  dt <- 0.01; tol <- 1e-3; tmax <- 10

  population <- Logistic()      # create a Logistic ODE object

  # Two ways of initializing the object
  # population <- init(population, c(x, vx, 0), r, K)
  init(population) <- list(initState = c(x, vx, 0),
                           r = r,
                           K = K)

  odeSolver <- Verlet(population)      # select the solver

  # Two ways of initializing the solver
  # odeSolver <- init(odeSolver, dt)
  init(odeSolver) <- dt

  population@odeSolver <- odeSolver
  # setSolver(population) <- odeSolver

  rowVector <- vector("list")
  i <- 1
  while (getTime(population) <= tmax) {
    rowVector[[i]] <- list(t = getTime(population),
                          s1 = getState(population)[1],
                          s2 = getState(population)[2])
    population <- doStep(population)
    i <- i + 1
  }
}

```

```

    }
    DT <- data.table::rbindlist(rowVector)
    return(DT)
  }
  # show solution
  solution <- LogisticApp()
  plot(solution)
  # ++++++ example: KeplerEnergyApp.R
  # Demonstration of the use of the Verlet ODE solver
  #

importFromExamples("KeplerEnergy.R") # source the class Kepler

KeplerEnergyApp <- function(verbose = FALSE) {
  # initial values
  x <- 1
  vx <- 0
  y <- 0
  vy <- 2 * pi
  dt <- 0.01
  tol <- 1e-3
  particle <- KeplerEnergy()

  # Two ways of initializing the ODE object
  # particle <- init(particle, c(x, vx, y, vy, 0))
  init(particle) <- c(x, vx, y, vy, 0)

  odeSolver <- Verlet(particle)

  # Two ways of initializing the solver
  # odeSolver <- init(odeSolver, dt)
  init(odeSolver) <- dt

  particle@odeSolver <- odeSolver
  initialEnergy <- getEnergy(particle)
  rowVector <- vector("list")
  i <- 1
  while (getTime(particle) <= 1.20) {
    rowVector[[i]] <- list(t = getState(particle)[5],
                          x = getState(particle)[1],
                          vx = getState(particle)[2],
                          y = getState(particle)[3],
                          vy = getState(particle)[4],
                          E = getEnergy(particle))

    particle <- doStep(particle)
    energy <- getEnergy(particle)
    i <- i + 1
  }
  DT <- data.table::rbindlist(rowVector)
  return(DT)
}

solution <- KeplerEnergyApp()

```

```

plot(solution)

# ++++++ application: Logistic.R
# Simulates the logistic equation
importFromExamples("Logistic.R")

# Run the application
LogisticApp <- function(verbose = FALSE) {
  x <- 0.1
  vx <- 0
  r <- 2      # Malthusian parameter (rate of maximum population growth)
  K <- 10.0   # carrying capacity of the environment
  dt <- 0.01; tol <- 1e-3; tmax <- 10

  population <- Logistic()      # create a Logistic ODE object

  # Two ways of initializing the object
  # population <- init(population, c(x, vx, 0), r, K)
  init(population) <- list(initState = c(x, vx, 0),
                           r = r,
                           K = K)

  odeSolver <- Verlet(population)      # select the solver

  # Two ways of initializing the solver
  # odeSolver <- init(odeSolver, dt)
  init(odeSolver) <- dt

  population@odeSolver <- odeSolver
  # setSolver(population) <- odeSolver

  rowVector <- vector("list")
  i <- 1
  while (getTime(population) <= tmax) {
    rowVector[[i]] <- list(t = getTime(population),
                          s1 = getState(population)[1],
                          s2 = getState(population)[2])
    population <- doStep(population)
    i <- i + 1
  }
  DT <- data.table::rbindlist(rowVector)
  return(DT)
}
# show solution
solution <- LogisticApp()
plot(solution)

```

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