

# Package ‘CancerInSilico’

November 25, 2022

**Type** Package

**Title** An R interface for computational modeling of tumor progression

**Version** 2.18.0

**Date** 2018-04-06

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**Description** The CancerInSilico package provides an R interface for running mathematical models of tumor progression and generating gene expression data from the results. This package has the underlying models implemented in C++ and the output and analysis features implemented in R.

**License** GPL-2

**Depends** R (>= 3.4), Rcpp

**Imports** methods, utils, graphics, stats

**LinkingTo** Rcpp, BH

**Suggests** testthat, knitr, rmarkdown, BiocStyle, Rtsne, viridis, rgl,  
gplots

**VignetteBuilder** knitr

**biocViews** ImmunoOncology, MathematicalBiology, SystemsBiology,  
CellBiology, BiomedicalInformatics, GeneExpression, RNASeq,  
SingleCell

**RoxygenNote** 6.1.1

**Encoding** UTF-8

**Collate** 'CellSimulation.R' 'GeneExpressionSimulation.R'  
'RcppExports.R' 'class-CellModel.R' 'class-CellType.R'  
'class-OffLatticeModel.R' 'class-DrasdoHohmeModel.R'  
'class-Drug.R' 'class-GeneExpressionParams.R' 'class-Pathway.R'  
'documentation.R'

**git\_url** <https://git.bioconductor.org/packages/CancerInSilico>

**git\_branch** RELEASE\_3\_16  
**git\_last\_commit** ad25a00  
**git\_last\_commit\_date** 2022-11-01  
**Date/Publication** 2022-11-25

## R topics documented:

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---

|                  |                                    |
|------------------|------------------------------------|
| calibratePathway | <i>calibrate pathway with data</i> |
|------------------|------------------------------------|

---

### Description

sets the min and max values for each gene in a pathway based on a data set

### Usage

```
calibratePathway(pathway, dataSet)
```

### Arguments

|         |                    |
|---------|--------------------|
| pathway | a 'Pathway' object |
| dataSet | reference data set |

### Value

pathway with min/max values for expression based on data set

---

|                |                       |
|----------------|-----------------------|
| CancerInSilico | <i>CancerInSilico</i> |
|----------------|-----------------------|

---

### Description

|          |                |
|----------|----------------|
| Package: | CancerInSilico |
| Type:    | Package        |
| Version: | 1.99.0         |
| Date:    | 2017-06-24     |
| License: | LGPL           |

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---

|                 |                  |
|-----------------|------------------|
| CellModel-class | <i>CellModel</i> |
|-----------------|------------------|

---

**Description**

The top-level CellModel class. All other cell model classes inherit from this in some way

**Slots**

`cells` A list object that describes the state of the cells at each time. The state representation depends on the type of model run, and is accessed by the function designed for each model type.

`initialNum` number of cells at time 0

`runTime` number of model hours to run the simulation

`density` initial density of cells

`boundary` keep cells within circular boundary

`syncCycles` start all cells in the beginning of interphase

`randSeed` random seed used for both R and C++ functions

`outputIncrement` how often simulation info is displayed

`recordIncrement` how often cell info is recorded (controls size of resulting CellModel object)

`timeIncrement` controls how fine the model timestep is

`cellTypes` list of CellType objects used in the model

`cellTypeInitFreq` initial frequency of cell types among cells

`drugs` list of Drug objects used in the model

---

|             |  |
|-------------|--|
| cellSummary | <i>summary of cell model at a given time</i> |
|-------------|--|

---

**Description**

summary of cell model at a given time

**Usage**

```
cellSummary(model, time)
```

```
## S4 method for signature 'CellModel'
cellSummary(model, time)
```

**Arguments**

`model` cell model object

`time` hour of the model to query

**Value**

string containing summary of model

**Examples**

```
data(SampleModels)
cellSummary(modDefault, modDefault@runTime)
```

---

|                |                 |
|----------------|-----------------|
| CellType-class | <i>CellType</i> |
|----------------|-----------------|

---

**Description**

The properties of a cell type

**Slots**

name the name of the cell type  
 size the relative size (volume) of the cell  
 minCycle minimum possible cell cycle length  
 cycleLength function that returns sample from distribution of cycle lengths

---

|              |  |
|--------------|--|
| checkDataSet | <i>verify gene expression data set is valid for this package</i> |
|--------------|--|

---

**Description**

checks a data set before it is used to calibrate the pathway values for min/max expression

**Usage**

```
checkDataSet(dataSet, genes)
```

**Arguments**

|         |  |
|---------|--|
| dataSet | matrix of gene expression data where row names are genes |
| genes   | names of all genes being simulated                       |

**Value**

no value is return, but errors/warnings are thrown related to potential problems in the data set

**Examples**

```
data(referenceGeneExpression)
```

---

DrasdoHohmeModel-class

*DrasdoHohmeModel*

---

**Description**

Implementation of an off-lattice cell-based model based on the work in Drasdo, Hohme (2003)

**Slots**

nG number of monte carlo steps between each growth trial

epsilon constant that controls the probability trails are accepted

delta controls distance over which short range interactions occur

---

Drug-class

*Drug*

---

**Description**

describes the properties of a drug

**Slots**

name name of drug

timeAdded the time at which this drug is added to the simulation

cycleLengthEffect effect this drug has on cell cycle length

---

GeneExpressionParams-class

*GeneExpressionParams*

---

**Description**

Parameters for simulating gene expression

**Slots**

sampleFreq how often to generate data  
 RNAseq generate RNA-seq data  
 singleCell generate single cell data  
 nCells number of cells to sample at each time point  
 nDummyGenes number of dummy genes  
 dummyDist function to determine expression of dummy genes  
 combineFUN function used to combine gene expression data  
 randSeed random seed  
 perError error for normal error model  
 bcvCommon error for voom error model  
 bcvDF degrees of freedom for voom error model  
 dropoutPresent whether to simulate dropout in single cell data  
 dropoutMid parameter for dropout distribution  
 dropoutShape parameter for dropout distribution

---

|              |  |
|--------------|--|
| getAxisAngle | <i>get cell axis angle at a given time</i> |
|--------------|--|

---

**Description**

get cell axis angle at a given time

**Usage**

```

getAxisAngle(model, time, cell)

## S4 method for signature 'OffLatticeModel'
getAxisAngle(model, time, cell)

```

**Arguments**

|       |                            |
|-------|----------------------------|
| model | cell model object          |
| time  | hour of the model to query |
| cell  | id of cell to query        |

**Value**

axis angle

**Examples**

```

data(SampleModels)
getAxisAngle(modDefault, modDefault@runTime, 1)

```

---

|               |   |
|---------------|---|
| getAxisLength | <i>get cell axis length at a given time</i> |
|---------------|---|

---

**Description**

get cell axis length at a given time

**Usage**

```
getAxisLength(model, time, cell)

## S4 method for signature 'OffLatticeModel'
getAxisLength(model, time, cell)
```

**Arguments**

|       |                            |
|-------|----------------------------|
| model | cell model object          |
| time  | hour of the model to query |
| cell  | id of cell to query        |

**Value**

axis length

**Examples**

```
data(SampleModels)
getAxisLength(modDefault, modDefault@runTime, 1)
```

---

|                 |                                       |
|-----------------|---------------------------------------|
| getCellDistance | <i>get distance between two cells</i> |
|-----------------|---------------------------------------|

---

**Description**

get distance between two cells

**Usage**

```
getCellDistance(model, time, cellA, cellB)

## S4 method for signature 'OffLatticeModel'
getCellDistance(model, time, cellA, cellB)
```



**Arguments**

|       |                            |
|-------|----------------------------|
| model | cell model object          |
| time  | hour of the model to query |
| cellA | id of cell to query        |
| cellB | id of cell to query        |

**Value**

distance between cellA and cellB

**Examples**

```
data(SampleModels)
getCellDistance(modDefault, modDefault@runTime, 1, 2)
```

---

|                     |  |
|---------------------|--|
| <i>getCellPhase</i> | <i>get phase of a cell at a given time</i> |
|---------------------|--|

---

**Description**

get phase of a cell at a given time

**Usage**

```
getCellPhase(model, time, cell)

## S4 method for signature 'OffLatticeModel'
getCellPhase(model, time, cell)
```

**Arguments**

|       |                            |
|-------|----------------------------|
| model | cell model object          |
| time  | hour of the model to query |
| cell  | id of cell to query        |

**Value**

cell phase

**Examples**

```
data(SampleModels)
getCellPhase(modDefault, modDefault@runTime, 1)
```

getCellType                    *get type of a cell at a given time*

---

**Description**

get type of a cell at a given time

**Usage**

```
getCellType(model, time, cell)

## S4 method for signature 'OffLatticeModel'
getCellType(model, time, cell)
```

**Arguments**

|       |                            |
|-------|----------------------------|
| model | cell model object          |
| time  | hour of the model to query |
| cell  | id of cell to query        |

**Value**

cell type

**Examples**

```
data(SampleModels)
getCellType(modDefault, modDefault@runTime, 1)
```

---

getCoordinates                *get coordinates of a cell at a given time*

---

**Description**

get coordinates of a cell at a given time

**Usage**

```
getCoordinates(model, time, cell)

## S4 method for signature 'OffLatticeModel'
getCoordinates(model, time, cell)
```

**Arguments**

|       |                            |
|-------|----------------------------|
| model | cell model object          |
| time  | hour of the model to query |
| cell  | id of cell to query        |

**Value**

pair of (x,y) coordinates

**Examples**

```
data(SampleModels)
getCoordinates(modDefault, modDefault@runTime, 1)
```

---

|                             |   |
|-----------------------------|---|
| <code>getCycleLength</code> | <i>get cycle length of a cell at a given time</i> |
|-----------------------------|---|

---

**Description**

get cycle length of a cell at a given time

**Usage**

```
getCycleLength(model, time, cell)

## S4 method for signature 'OffLatticeModel'
getCycleLength(model, time, cell)
```

**Arguments**

|       |                            |
|-------|----------------------------|
| model | cell model object          |
| time  | hour of the model to query |
| cell  | id of cell to query        |

**Value**

cycle length in hours

**Examples**

```
data(SampleModels)
getCycleLength(modDefault, modDefault@runTime, 1)
```

---

|            |   |
|------------|---|
| getDensity | <i>get density of the cell population at a given time</i> |
|------------|---|

---

**Description**

get density of the cell population at a given time

**Usage**

```
getDensity(model, time)
```

```
## S4 method for signature 'OffLatticeModel'  
getDensity(model, time)
```

**Arguments**

|       |                            |
|-------|----------------------------|
| model | cell model object          |
| time  | hour of the model to query |

**Value**

density

**Examples**

```
data(SampleModels)  
getDensity(modDefault, modDefault@runTime)
```

---

|                 |   |
|-----------------|---|
| getLocalDensity | <i>get neighborhood density around a cell at a given time</i> |
|-----------------|---|

---

**Description**

get neighborhood density around a cell at a given time

**Usage**

```
getLocalDensity(model, time, cell, radius)
```

```
## S4 method for signature 'OffLatticeModel'  
getLocalDensity(model, time, cell, radius)
```

**Arguments**

|        |  |
|--------|--|
| model  | cell model object                        |
| time   | hour of the model to query               |
| cell   | id of cell to query                      |
| radius | distance to search for neighboring cells |

**Value**

density

**Examples**

```
data(SampleModels)
getLocalDensity(modDefault, modDefault@runTime, 1, 3.3)
```

---

|                               |   |
|-------------------------------|---|
| <code>getNumberOfCells</code> | <i>get number of cells in the model at a given time</i> |
|-------------------------------|---|

---

**Description**

get number of cells in the model at a given time

**Usage**

```
getNumberOfCells(model, time)

## S4 method for signature 'OffLatticeModel'
getNumberOfCells(model, time)
```

**Arguments**

|       |                            |
|-------|----------------------------|
| model | cell model object          |
| time  | hour of the model to query |

**Value**

number of cells

**Examples**

```
data(SampleModels)
getNumberOfCells(modDefault, modDefault@runTime)
```

---

|           |  |
|-----------|--|
| getRadius | <i>get cell radius at a given time</i> |
|-----------|--|

---

**Description**

get cell radius at a given time

**Usage**

```
getRadius(model, time, cell)

## S4 method for signature 'OffLatticeModel'
getRadius(model, time, cell)
```

**Arguments**

|       |                            |
|-------|----------------------------|
| model | cell model object          |
| time  | hour of the model to query |
| cell  | id of cell to query        |

**Value**

radius of cell

**Examples**

```
data(SampleModels)
getRadius(modDefault, modDefault@runTime, 1)
```

---

|                    |  |
|--------------------|--|
| getTrialAcceptRate | <i>get rate of growth acceptance of a given cell at a given time</i> |
|--------------------|--|

---

**Description**

get rate of growth acceptance of a given cell at a given time

**Usage**

```
getTrialAcceptRate(model, time, cell)

## S4 method for signature 'OffLatticeModel'
getTrialAcceptRate(model, time, cell)
```

**Arguments**

|       |                            |
|-------|----------------------------|
| model | cell model object          |
| time  | hour of the model to query |
| cell  | id of cell to query        |

**Value**

acceptance rate

**Examples**

```
data(SampleModels)
getTrialAcceptRate(modDefault, modDefault@runTime, 1)
```

---

initialize,CellModel-method

*Constructor for CellModel*

---

**Description**

Constructor for CellModel

**Usage**

```
## S4 method for signature 'CellModel'
initialize(.Object, initialNum, runTime, density,
  boundary = 1, syncCycles = FALSE, randSeed = 0,
  outputIncrement = 4, recordIncrement = 0.1, timeIncrement = 0.001,
  cellTypes = c(new("CellType", name = "DEFAULT")),
  cellTypeInitFreq = c(1), drugs = list(), ...)
```

**Arguments**

|                 |  |
|-----------------|--|
| .Object         | CellModel object   |
| initialNum      | initial number of cells                                  |
| runTime         | run time of the model in hours                           |
| density         | initial density of the cell population                   |
| boundary        | impose a physical boundary on the cells                  |
| syncCycles      | synchronization all cells to the same point in the cycle |
| randSeed        | random seed  |
| outputIncrement | how often (model hours) to print simulation status       |
| recordIncrement | how often (model hours) to record cell information       |

|                  |  |
|------------------|--|
| timeIncrement    | internal time step (model hours) used by the model |
| cellTypes        | list of CellType objects                           |
| cellTypeInitFreq | initial proportions of all cell types              |
| drugs            | list of Drug objects                               |
| ...              | model specific parameters                          |

**Value**

initialized cell model object

---

*initialize,DrasdoHohmeModel-method*  
*DrasdoHohmeModel Constructor*

---

**Description**

DrasdoHohmeModel Constructor

**Usage**

```
## S4 method for signature 'DrasdoHohmeModel'
initialize(.Object, nG = 28, epsilon = 10,
  delta = 0.2, ...)
```

**Arguments**

|         |                                   |
|---------|-----------------------------------|
| .Object | DrasdoHohmeModel object           |
| nG      | number of trials per growth trial |
| epsilon | model parameter                   |
| delta   | small scale interaction distance  |
| ...     | extra parameters                  |

**Value**

initialized cell model



---

```
initialize,OffLatticeModel-method
      Off-Lattice Model Constructor
```

---

**Description**

Off-Lattice Model Constructor

**Usage**

```
## S4 method for signature 'OffLatticeModel'
initialize(.Object, maxTranslation = 0.1,
          maxRotation = 0.3, ...)
```

**Arguments**

|                |                                  |
|----------------|----------------------------------|
| .Object        | OffLatticeModel object           |
| maxTranslation | maximum movement of cell         |
| maxRotation    | maximim rotation of mitosis cell |
| ...            | model specific parameters        |

**Value**

initialized cell model

---

```
inSilicoCellModel      Simulates Cell Model
```

---

**Description**

Simulates Cell Model

**Usage**

```
inSilicoCellModel(initialNum, runTime, density,
                  modelType = "DrasdoHohme", ...)
```

**Arguments**

|            |  |
|------------|--|
| initialNum | how many cells initially                                   |
| runTime    | how long the simulation runs in real cellular time (hours) |
| density    | initial density of cell population                         |
| modelType  | the name of the cell-based model to use                    |
| ...        | model specific parameters (depends on modelType)           |

**Details**

This function provides a centralized R interface to run c++ code for cell-based models implemented in this package. Standard parameters, as well as model-specific parameters, are passed in to this function along with a model name. This function then runs the model and returns a CellModel object containing all of the information from the model. This object can then be accessed with various functions designed to interact with the class. To see a list of available functions, there is a show() command implemented for CellModel objects.

**Value**

A CellModel containing all info from the model run

**Examples**

```
inSilicoCellModel(initialNum=1, runTime=8, density=0.1)
```

---

inSilicoGeneExpression

*simulate gene expression data*

---

**Description**

simulate gene expression data for a set of pathways, using the behavior of a CellModel as the basis for the simulation

**Usage**

```
inSilicoGeneExpression(model, pathways,  
  params = new("GeneExpressionParams"))
```

**Arguments**

|          |                             |
|----------|-----------------------------|
| model    | a CellModel object          |
| pathways | list of genes pathways      |
| params   | GeneExpressionParams object |

**Value**

list of pathway activity and gene expression

---

|                  |  |
|------------------|--|
| inSilicoPathways | <i>This data contains the list of gene targets of modeled signaling pathways</i> |
|------------------|--|

---

**Description**

This data contains the list of gene targets of modeled signaling pathways

**Usage**

```
inSilicoPathways
```

**Details**

List of gene targets for GtoM, GtoS, and Growth factor pathways modeled in CancerInSilico. GtoM represents genes associated with the G to M checkpoint of the cell cycle collected from PID pathways PI3KCI\_AKT, TNF, TGFBR, and RB1 in MSigDB v5.1. GtoS represented genes associated with the G to S checkpoint of the cell cycle collected from E2F target genes in PID and hallmark genesets from MSigDb v5.1 and experimentally validated targets in TRANSFAC professional 2014. Growth represents the targets of transcription factors resulting from EGFR activation (STAT1, STAT3, STAT5, Elk-1, Myc, NF-kappaB, and RelA) from the TRANSFAC professional database 2014 as described in Fertig et al, 2012.

**Value**

List of gene targets for GtoM, GtoS, and Growth factor pathways.

**References**

Subramanian, Tamayo, et al, PNAS, 102:155545, 2005; Matys et al, Nuc Ac Res, 34:D108, 2006; and Fertig et al, BMC Genomics, 13:160, 2012.

---

|                 |  |
|-----------------|--|
| interactivePlot | <i>plot the cell population and interactively scroll through time points</i> |
|-----------------|--|

---

**Description**

plot the cell population and interactively scroll through time points

**Usage**

```
interactivePlot(model)

## S4 method for signature 'CellModel'
interactivePlot(model)
```

**Arguments**

model            cell model object

**Value**

plot

---

modCellTypes            *sample cell model*

---

**Description**

sample cell model

**Usage**

modCellTypes

---

modDefault            *sample cell model*

---

**Description**

sample cell model

**Usage**

modDefault

---

modDrugs            *sample cell model*

---

**Description**

sample cell model

**Usage**

modDrugs

---

|                |                          |
|----------------|--------------------------|
| modHighDensity | <i>sample cell model</i> |
|----------------|--------------------------|

---

**Description**

sample cell model

**Usage**

modHighDensity

---

|             |                          |
|-------------|--------------------------|
| modLargeRun | <i>sample cell model</i> |
|-------------|--------------------------|

---

**Description**

sample cell model

**Usage**

modLargeRun

---

|            |                          |
|------------|--------------------------|
| modLongRun | <i>sample cell model</i> |
|------------|--------------------------|

---

**Description**

sample cell model

**Usage**

modLongRun

---

|                       |                        |
|-----------------------|------------------------|
| OffLatticeModel-class | <i>OffLatticeModel</i> |
|-----------------------|------------------------|

---

**Description**

General description of an off-lattice cell-based model. not quite a full implementation, but contains much of the necessary structure for models of this type

**Slots**

maxTranslation the largest distance the center of a cell can move

maxRotation the largest angle a cell can rotate

---

 Pathway-class

*Pathway Class*


---

**Description**

Describes the basic properties of a gene pathway

**Usage**

```
## S4 method for signature 'Pathway'
initialize(.Object, ...)
```

**Arguments**

|         |                                 |
|---------|---------------------------------|
| .Object | Pathway object                  |
| ...     | extra arguments for constructor |

**Details**

expressionScale is a function that accepts three arguments: model, cell, and time. It should return a number in [0,1] that describes how active the genes are in this pathway for a given cell in the model at a given time. In bulk data, the pathway activity is averaged and transformed by  $1 / (1 + \exp(-k * (x - M)))$  where  $k = \text{transformSlope}$  and  $M = \text{transformMidpoint}$ . The scale determines how expressed genes in this pathway are. i.e. and scale of 0 means all genes will have minExpression value and a scale of 1 means all genes will have maxExpression value. In between these values the gene expression scales linearly.

**Value**

constructed object

**Slots**

|                   |  |
|-------------------|--|
| genes             | names of genes in the pathway  |
| expressionScale   | function describing how this pathway is affected by the state of the model |
| minExpression     | minimum expression value for each gene (vector)                            |
| maxExpression     | maximum expression value for each gene (vector)                            |
| transformSlope    | parameter for transforming bulk data                                       |
| transformMidpoint | parameter for transforming bulk data                                       |

---

plotCells                    *plot cell population at a given time*

---

**Description**

plot cell population at a given time

**Usage**

```
plotCells(model, time)

## S4 method for signature 'OffLatticeModel'
plotCells(model, time)
```

**Arguments**

|       |                            |
|-------|----------------------------|
| model | cell model object          |
| time  | hour of the model to query |

**Value**

plot

**Examples**

```
data(SampleModels)
plotCells(modDefault, modDefault@runTime)
```

---

pwyContactInhibition    *sample pathway*

---

**Description**

sample pathway

**Usage**

```
pwyContactInhibition
```

---

pwyGrowth                      *sample pathway*

---

**Description**

sample pathway

**Usage**

pwyGrowth

---

pwyMitosis                      *sample pathway*

---

**Description**

sample pathway

**Usage**

pwyMitosis

---

pwySPhase                      *sample pathway*

---

**Description**

sample pathway

**Usage**

pwySPhase

---

referenceGeneExpression  
*gene expression data for genes in sample pathways*

---

**Description**

gene expression data for genes in sample pathways

**Usage**

referenceGeneExpression



---

|     |                         |
|-----|-------------------------|
| run | <i>run a cell model</i> |
|-----|-------------------------|

---

**Description**

run a cell model

**Usage**

```
run(model)
```

```
## S4 method for signature 'DrasdoHohmeModel'  
run(model)
```

**Arguments**

model            cell model object

**Value**

cell model object with simulation info

**Examples**

```
data(SampleModels)  
run(modDefault)
```

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