Getting started with RLumCarlo

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Scope

RLumCarlo is collection of energy-band models to simulate luminescence signals using Monte-Carlo (MC) methods. This document aims at providing an overview and a brief introduction to RLumCarlo.

The models in RLumCarlo

The following tables lists the models implemented in RLumCarlo along with the **R** function call and the corresponding R (*.R) and C++ (*.cpp) files. The modelling takes place in the C++ functions which are wrapped by the R functions with a similar name. If you, however, want to cross-check the code, you should inspect files with the ending '.cpp'.

MODEL.NAME	R.CALL	FILES
MC_CW_IRSL_LOC	run_MC_CW_IRSL_LOC()	R/run_MC_CW_IRSL_LOC.R src/MC_C_MC_CW_IRSL_LOC.cpp
MC_CW_IRSL_TUN	run_MC_CW_IRSL_TUN()	R/run_MC_CW_IRSL_TUN.R src/MC_C_MC_CW_IRSL_TUN.cpp
MC_CW_OSL_DELOC	run_MC_CW_OSL_DELOC()	R/run_MC_CW_OSL_DELOC.R src/MC_C_MC_CW_OSL_DELOC.cpp
MC_ISO_DELOC	run_MC_ISO_DELOC()	R/run_MC_ISO_DELOC.R src/MC_C_MC_ISO_DELOC.cpp
MC_ISO_LOC	run_MC_ISO_LOC()	R/run_MC_ISO_LOC.R src/MC_C_MC_ISO_LOC.cpp
MC_ISO_TUN	run_MC_ISO_TUN()	R/run_MC_ISO_TUN.R src/MC_C_MC_ISO_TUN.cpp
MC_LM_OSL_DELOC	run_MC_LM_OSL_DELOC()	R/run_MC_LM_OSL_DELOC.R src/MC_C_MC_LM_OSL_DELOC.cpp
MC_LM_OSL_LOC	run_MC_LM_OSL_LOC()	R/run_MC_LM_OSL_LOC.R src/MC_C_MC_LM_OSL_LOC.cpp
MC_LM_OSL_TUN	run_MC_LM_OSL_TUN()	R/run_MC_LM_OSL_TUN.R src/MC_C_MC_LM_OSL_TUN.cpp
MC_TL_DELOC	run_MC_TL_DELOC()	R/run_MC_TL_DELOC.R src/MC_C_MC_TL_DELOC.cpp
MC_TL_LOC	run_MC_TL_LOC()	R/run_MC_TL_LOC.R src/MC_C_MC_TL_LOC.cpp
MC_TL_TUN	run_MC_TL_TUN()	R/run_MC_TL_TUN.R src/MC_C_MC_TL_TUN.cpp

Each model can be run by calling one of the **R** functions starting with `run_`. Currently three different model

types (TUN: tunneling, LOC: localised transition, DELOC: delocalised transition) are implemented for the stimulation types TL, IRSL, LM-OSL, and ISO (isothermal). Please note that each model has different parameters and requirements.

The following table summarizes the parameters used in the implemented MC models along with their physical meaning, units and the range of realistic values. This range represents just a rough guideline and might be exceeded for particular cases.

Stimulation mode	Parameter	Parameter description	Unit	Realistic values
Delocalized TL	E	Thermal activation energy of the trap	eV	0.5–3
	s	Frequency factor of the trap	1/s	1E8–1E16
	times	Sequence of temperature steps for simulation	°C	0–700
	clusters	Number of MC runs	1	1E1–1E4
	N_e	Total number of electron traps available	1	2–1E5
	n_filled	Number of filled electron traps at the beginning of the simulation	1	1–1E5
	R	Delocalized retrapping ratio	1	0–1
Delocalized CW-IRSL	A	Optical excitation rate from trap to conduction band	1/s	1E-3–1
	times	Sequence of time steps for simulation	s	0–500
	clusters	Number of MC runs	1	1E1–1E4
	N_e	Total number of electron traps available	1	2–1E5
	n_filled	Number of filled electron traps at the beginning of the simulation	1	1–1E5
	R	Delocalized retrapping ratio	1	0–1
Delocalized ISO	E	Thermal activation energy of the trap	eV	0.5–3
	s	Frequency factor of the trap	1/s	1E8–1E16
	T	Temperature	°C	20–300
	times	Sequence of time steps for simulation	s	0–1000
	clusters	Number of MC runs	1	1E1–1E4
	N_e	Number of electrons	1	2–1E5
	n_filled	Number of filled electron traps at the beginning of the simulation	1	1–1E5
	R	Delocalized retrapping ratio	1	0–1
Delocalized LM-OSL	A	Optical excitation rate from trap to conduction band	1/s	1E-3–1
	times	Sequence of time steps for simulation	s	0–3000
	clusters	Number of MC runs	1	1E1–1E4
	N_e	Total number of electron traps available	1	2–1E5
	n_filled	Number of filled electron traps at the beginning of the simulation	1	1–1E5
	R	Delocalized retrapping ratio	1	0–1
Localized TL	E	Thermal activation energy of the trap	eV	0.5–3
	s	Frequency factor of the trap	1/s	1E8–1E16
	times	Sequence of temperature steps for simulation	°C	0–700
	clusters	Number of MC runs	1	1E1–1E4

	n_filled	Number of filled electron traps at the beginning of the simulation	1	1–1E5
	r	Localized retrapping ratio	1	0–1E5
Localized CW-IRSL	A	Excitation rate from ground state of the trap to the excited state	1/s	1E-3–1
	times	Sequence of time steps for simulation	s	0–500
	clusters	Number of MC runs	1	1E1–1E4
	n_filled	Number of filled electron traps at the beginning of the simulation	1	1–1E5
	r	Localized retrapping ratio	1	0–1E5
Localized ISO	E	Thermal activation energy of the trap	eV	0.5–3
	s	Frequency factor of the trap	1/s	1E8–1E16
	T	Temperature	°C	20–300
	times	Sequence of time steps for simulation	s	0–1000
	clusters	Number of MC runs	1	1E1–1E4
	n_filled	Number of filled electron traps at the beginning of the simulation	1	1–1E5
	r	Localized retrapping ratio	1	0–1E5
Localized LM-OSL	A	Excitation rate from ground state of the trap to the excited state	1/s	1E-3–1
	times	Sequence of time steps for simulation	s	0–3000
	clusters	Number of MC runs	1	1E1–1E4
	n_filled	Number of filled electron traps at the beginning of the simulation	1	1–1E5
	r	Localized retrapping ratio	1	0–1E5
TL with tunneling recombination	E	Thermal activation energy of the trap	eV	0.5–3
	s	Frequency factor of the trap	1/s	1E8–1E16
	rho	Density of recombination centers (defined as ρ' in Huntley 2006)	1	1E-7–1E-4
	r_c	Critical distance (>0) that is to be inserted if the sample has been thermally and/or optically pretreated, so that the electron-hole pairs within r_c have already recombined	1	0–2
	times	Sequence of temperature steps for simulation	°C	0–700
	clusters	Number of MC runs	1	1E1–1E4
	N_e	Total number of electron traps available	1	2–1E5
	delta.r	Increments of the unitless distance parameter r	1	1E-3–1E-1
CW-IRSL with tunneling recombination	A	Excitation rate from ground state of the trap to the excited state	1/s	1E-3–1
	rho	Density of recombination centers (defined as ρ' in Huntley 2006)	1	1E-7–1E-4
	times	Sequence of time steps for simulation	s	0–500
	clusters	Number of MC runs	1	1E1–1E4
	N_e	Total number of electron traps available	1	2–1E5

	r_c	Critical distance (>0) that is to be inserted if the sample has been thermally and/or optically pretreated, so that the electron-hole pairs within r_c have already recombined	1	0–2
	delta.r	Increments of the unitless distance parameter r	1	1E-3–1E-1
ISO with tunneling recombination	E	Thermal activation energy of the trap	eV	0.5–3
	s	Frequency factor of the trap	1/s	1E8–1E16
	T	Temperature	°C	20–300
	rho	Density of recombination centers (defined as ρ' in Huntley 2006)	1	1E-7–1E-4
	times	Sequence of time steps for simulation	s	0–1000
	clusters	Number of MC runs	1	1E1–1E4
	N_e	Total number of electron traps available	1	2–1E5
	r_c	Critical distance (>0) that is to be inserted if the sample has been thermally and/or optically pretreated, so that the electron-hole pairs within r_c have already recombined	1	0–2
	delta.r	Increments of the unitless distance parameter r	1	1E-3–1E-1
LM-OSL with tunneling recombination	A	Excitation rate from ground state of the trap to the excited state	1/s	1E-3–1
	rho	Density of recombination centers (defined as ρ' in Huntley 2006)	1	1E-7–1E-4
	times	Sequence of time steps for simulation	s	0–3000
	clusters	Number of MC runs	1	1E1–1E4
	N_e	Total number of electron traps available	1	2–1E5
	r_c	Critical distance (>0) that is to be inserted if the sample has been thermally and/or optically pretreated, so that the electron-hole pairs within r_c have already recombined	1	0–2
	delta.r	Increments of the unitless distance parameter r	1	1E-3–1E-1

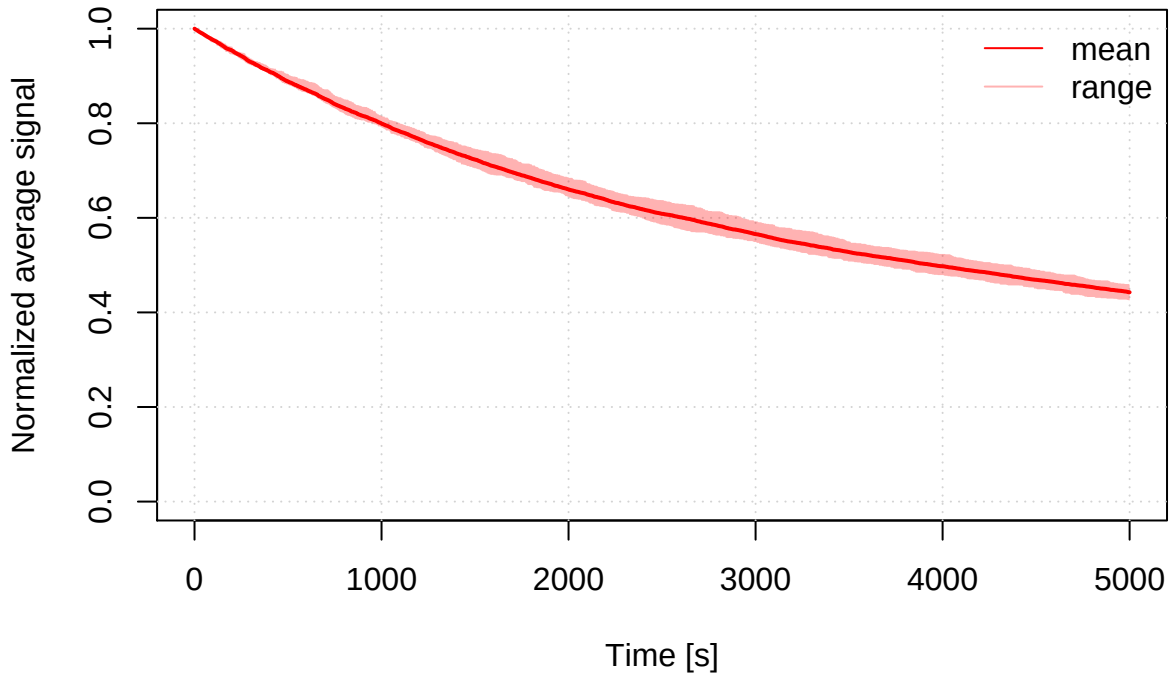
Examples

Example 1: A first example

The first examples simulates an iso-thermal curve using the tunneling model. Returned are either the simulated signal or the estimated remaining charges. The Function `plot_RLumCarlo()` provides an easy way to visualise the modelling results.

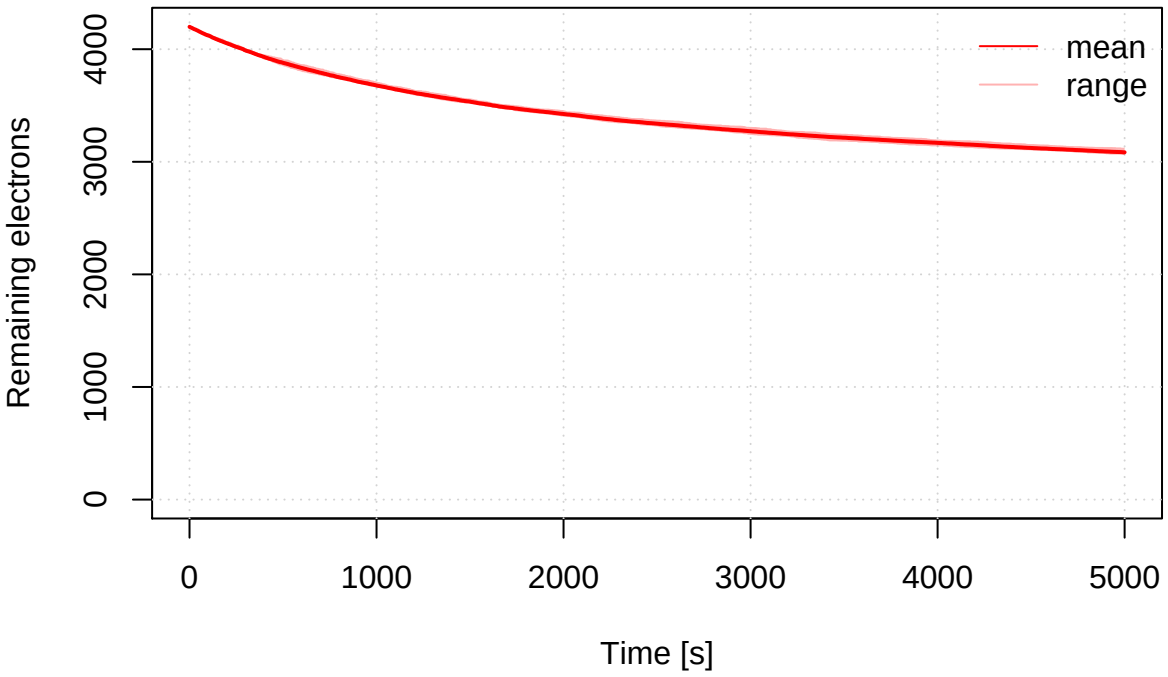
Modell the signal

```
results <- run_MC_ISO_TUN(
  E = 1.2,
  s = 1e10,
  T = 200,
  rho = 0.007,
  times = seq(0, 5000)
) %T>%
  plot_RLumCarlo(norm = TRUE, legend = TRUE)
```



Modell remaining charges

```
results <- run_MC_ISO_TUN(
  E = 1.2,
  s = 1e10,
  T = 200,
  rho = 0.007,
  times = seq(0, 5000),
  output = "remaining_e"
) %T>%
  plot_RLumCarlo(
    legend = TRUE,
    ylab = "Remaining electrons"
    )
```



Understanding the numerical output

The modelling output is an object of class `RLumCarlo_Model_Output`, which is basically a list consisting of an array and a vector.

```
str(results)
```

```
## List of 2
##  $ signal: num [1:5001, 1:21, 1:10] 200 200 200 200 200 197 196 196 196 196 ...
##   ..- attr(*, "dimnames")=List of 3
##   .. ..$ : NULL
##   .. ..$ : NULL
##   .. ..$ : NULL
##  $ time  : int [1:5001] 0 1 2 3 4 5 6 7 8 9 ...
##  - attr(*, "class")= chr "RLumCarlo_Model_Output"
##  - attr(*, "model")= chr "run_MC_ISO_TUN"
```

While this represents the full modelling output results, its interpretation might be less straight forward and the user may want to condense the information via `summary()`. The function `summary()` is also used internally by the function `plot_RLumCarlo()`.

```
df <- summary(results)
```

```
##       time           mean          y_min          y_max
##  Min.   :   0   Min.   :3084   Min.   :3060   Min.   :3125
##  1st Qu.:1250   1st Qu.:3190   1st Qu.:3159   1st Qu.:3224
##  Median :2500   Median :3338   Median :3314   Median :3375
##  Mean   :2500   Mean   :3424   Mean   :3399   Mean   :3457
##  3rd Qu.:3750   3rd Qu.:3599   3rd Qu.:3577   3rd Qu.:3632
##  Max.   :5000   Max.   :4199   Max.   :4197   Max.   :4200
##        sd              var
##  Min.   : 0.8756   Min.   :  0.7667
##  1st Qu.:15.9360   1st Qu.:253.9556
##  Median :18.0012   Median :324.0444
```

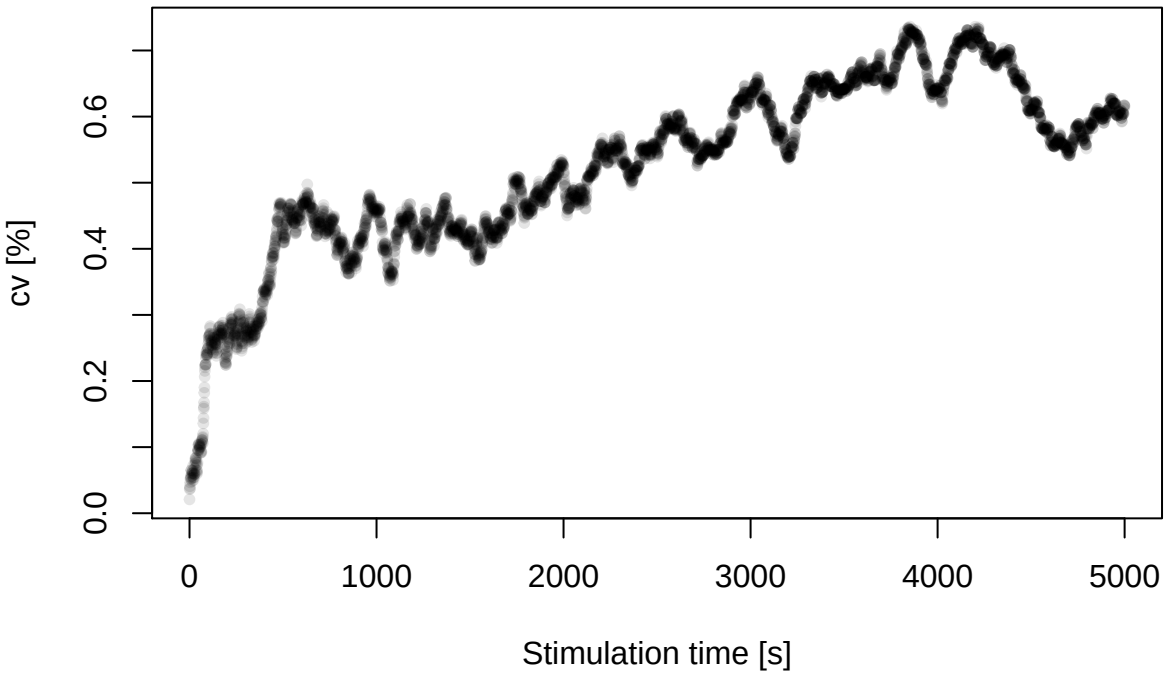
```
##  Mean   :17.6238   Mean   :322.5932
##  3rd Qu.:20.2989   3rd Qu.:412.0444
##  Max.   :23.4132   Max.   :548.1778
```

```
head(df)
```

```
##   time   mean y_min y_max       sd       var
## 1    0 4198.9  4197  4200 0.875595 0.7666667
## 2    1 4197.9  4195  4200 1.523884 2.3222222
## 3    2 4197.4  4194  4199 1.712698 2.9333333
## 4    3 4196.4  4194  4199 1.577621 2.4888889
## 5    4 4195.6  4192  4198 1.955050 3.8222222
## 6    5 4194.4  4190  4197 2.170509 4.7111111
```

The call summarises the modelling results and returns a terminal output and a `data.frame` with, e.g., the mean or the standard deviation, which can be used to create plots for further insight. For instance, the stimulation time agains the relative standard deviation:

```
plot(
  x = df$time,
  y = (df$sd / df$mean) * 100,
  pch = 20,
  col = rgb(0,0,0,.1),
  xlab = "Stimulation time [s]",
  ylab = "cv [%]"
)
```



Example 2: Combining two plots

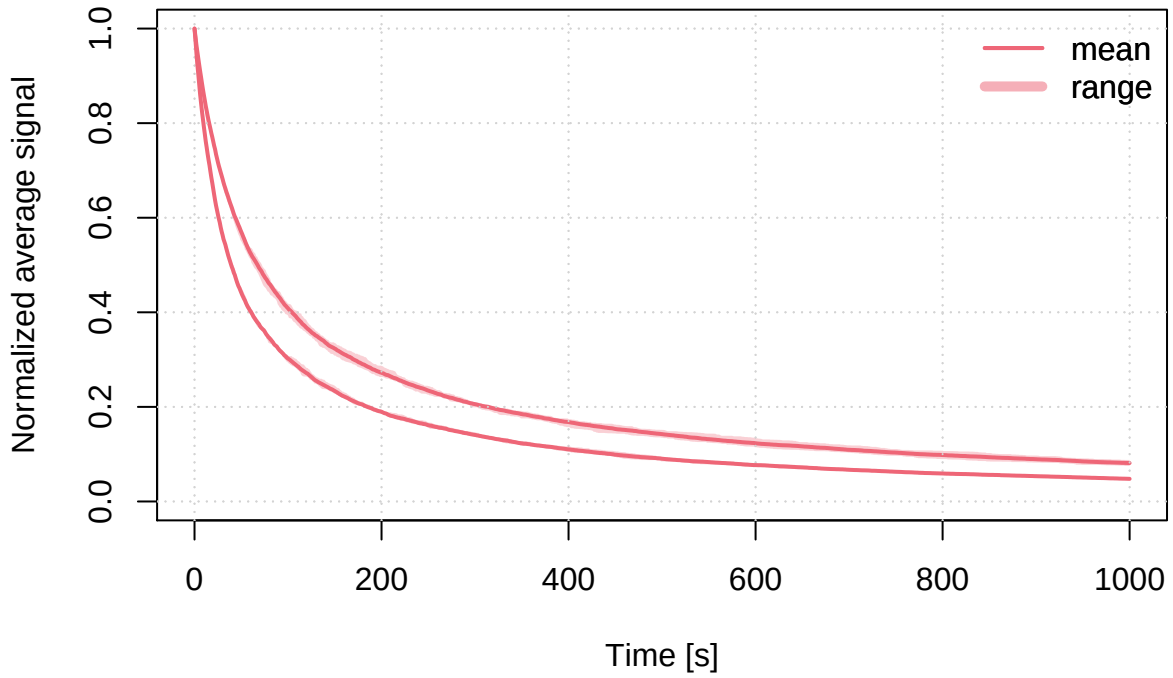
The following example uses continuous wave (CW) infrared light stimulation (IRSL), and combines two plots in one single plot window.

```
times <- seq(0, 1000)

## Run MC simulation
```

```r
run_MC_CW_IRSL_TUN(A = 0.12, rho = 0.003, times = times) %>%
  plot_RLumCarlo(norm = TRUE, legend = TRUE)

run_MC_CW_IRSL_TUN(A = 0.21, rho = 0.003, times = times) %>%
  plot_RLumCarlo(norm = TRUE, add = TRUE)
```

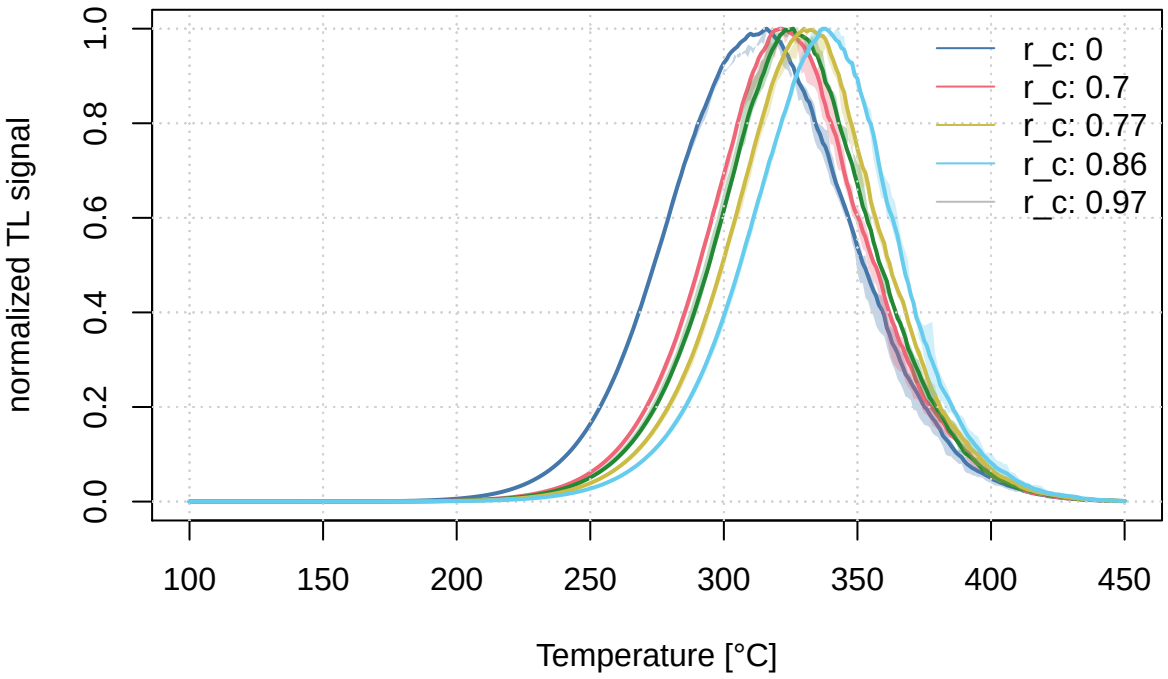


Example 3: Testing different parameters

The example above can be further extended to test the effect of different parameters. Contrary to the example above, here the results are stored in a `list` and `plot_RLumCarlo()` is called only one time.

```r
s <- 3.5e12
rho <- 0.015
E <- 1.45
r_c <- c(0,0.7,0.77,0.86, 0.97)
times <- seq(100, 450) # time = temperature
results <- lapply(r_c, function(x) {
  run_MC_TL_TUN(
    s = s,
    E = E,
    rho = rho,
    r_c = x,
    times = times
  )

})
```


normalized TL signal
0.0
0.2
0.4
0.6
0.8
1.0
100
150
200
250
300
350
400
450
Temperature [°C]
r_c: 0
r_c: 0.7
r_c: 0.77
r_c: 0.86
r_c: 0.97