Getting started with RLumCarlo

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RLumCarlo: v0.1.0.9000.120 | Last modified: 2019-11-03

Scope

RLumCarlo is a collection of energy-band models to simulate luminescence signals using Monte-Carlo (MC) methods for various stimulation modes. This document aims at supplementing the package documentation and elaborates the package examples.

The models in RLumCarlo

The following table lists all 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 is run by calling one of the **R** functions starting with `run_`. Currently, three different model types (TUN: tunnelling, 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.

RLumCarlo model parameters and variables

The following table summarises 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 time steps for simulation	s	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 time steps for simulation	s	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 time steps for simulation	s	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

The following examples exemplify the capacity of RLumCarlo, by using an example with longer simulation times than allowed for the standard package examples, which aim at a functionality test.

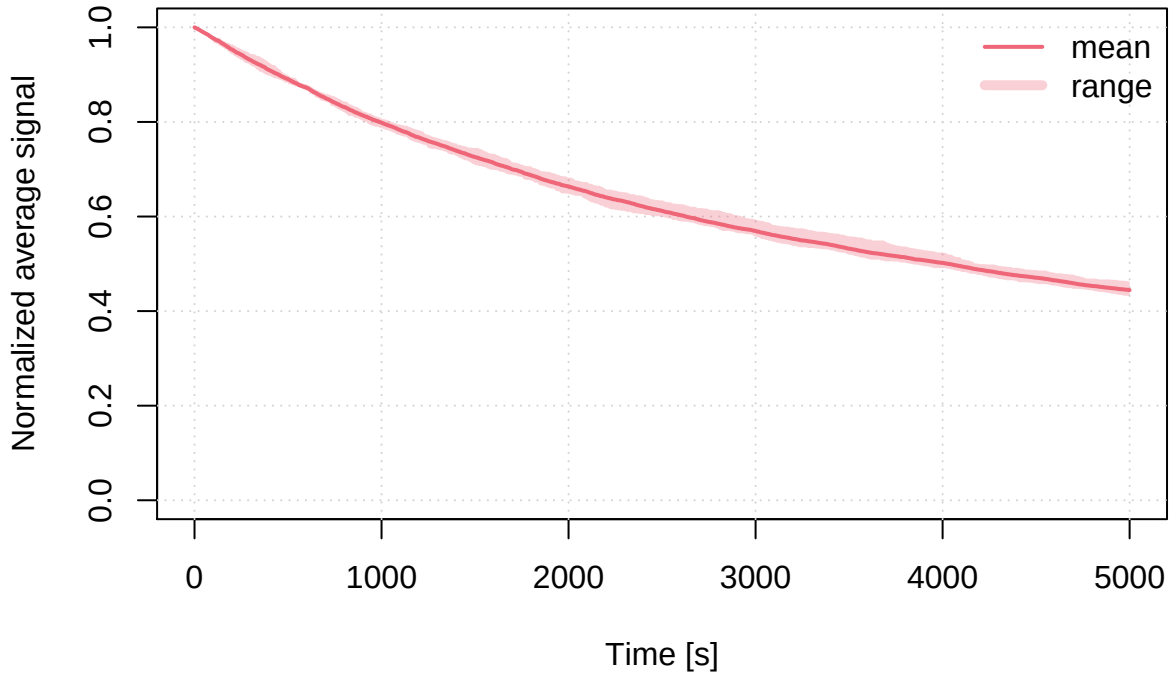
Example 1: A first example

The first examples iso-thermal curve using the tunnelling model (other models work similar). Returned are either the simulated signal or the estimated remaining charges. The Function `plot_RLumCarlo()` provides an easy way to visualise the modelling results and is here called using the tee operator `%T>` from the package `magrittr` (which is imported by RLumCarlo). Simulation results are stored in the object `results` while, at the same time, piped to the function `plot_RLumCarlo()` for the output visualisation.

Model the signal

The most obvious modelling output is the luminescence signal itself, our example below simulates an iso-thermal (ITL) signal for a temperature (`T`) of 200 °C over 5,000 s using a tunnelling transition model. Trap parameters are E = 1.2 (eV) for the trap depth and a frequency factor for 1×10^{10} (1/s). The parameter `rho` (ρ) defines the recombination centre density.

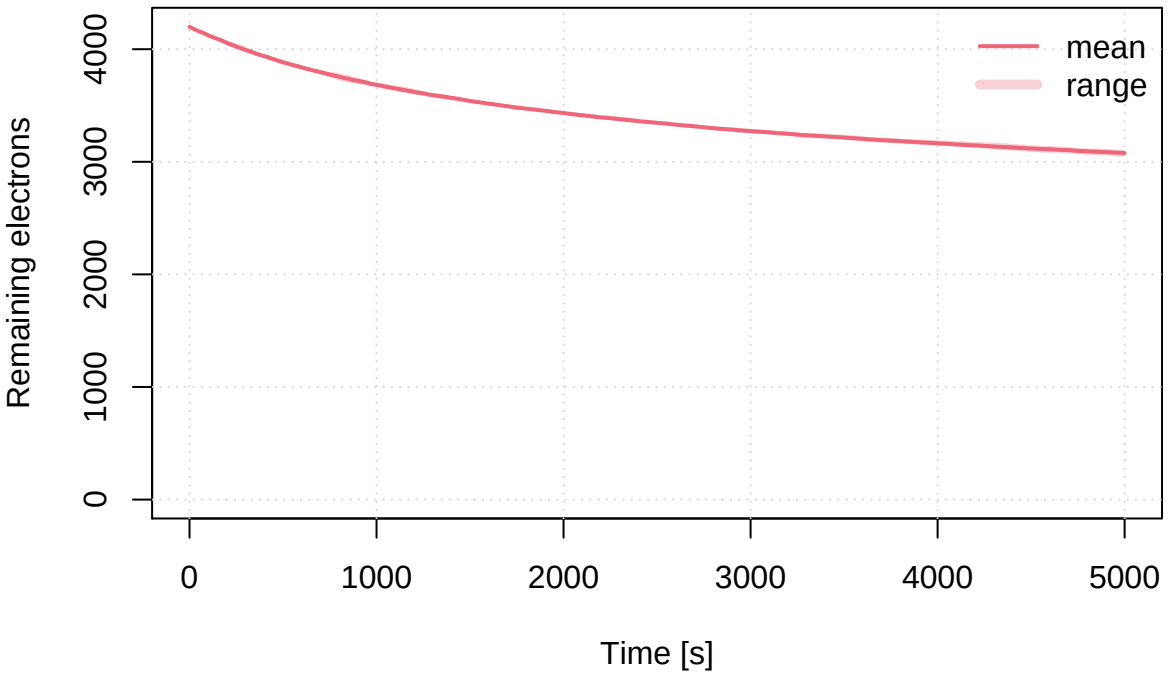
```r
results <- run_MC_ISO_TUN(
  E = 1.2,
  s = 1e10,
  T = 200,
  rho = 0.007,
  times = seq(0, 5000)
) %T>%
  plot_RLumCarlo(norm = TRUE, legend = TRUE)
```



Model remaining charges

The first example can be slightly varified. Instead of the luminescence signal, the variant returns the number of remaining electrons in the trap.

```r
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

In both cases 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] 200 200 200 200 199 199 199 199 196 195 ...
##   ..- 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.   :3078   Min.   :3044   Min.   :3106
##  1st Qu.:1250   1st Qu.:3188   1st Qu.:3167   1st Qu.:3210
##  Median :2500   Median :3346   Median :3335   Median :3364
##  Mean   :2500   Mean   :3427   Mean   :3407   Mean   :3448
##  3rd Qu.:3750   3rd Qu.:3607   3rd Qu.:3587   3rd Qu.:3628
##  Max.   :5000   Max.   :4199   Max.   :4195   Max.   :4200
##        sd              var
##  Min.   : 1.135   Min.   :  1.289
##  1st Qu.:10.607   1st Qu.:112.500
##  Median :13.760   Median :189.344
```

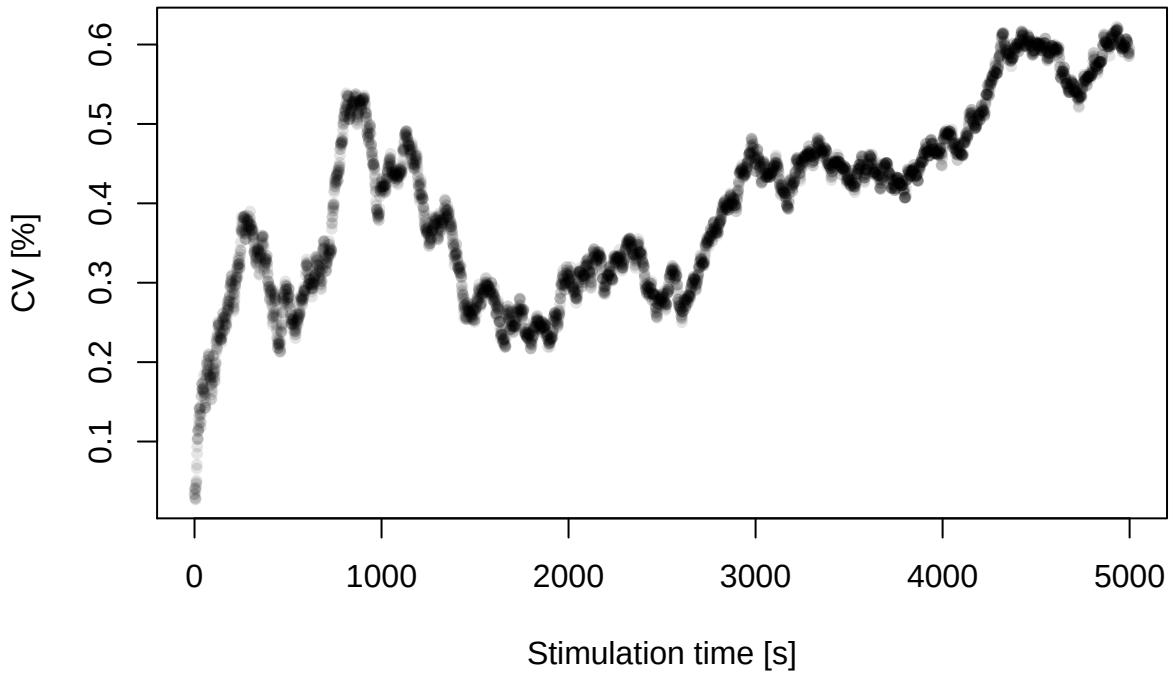
```
##  Mean   :13.435   Mean   :191.681
##  3rd Qu.:15.626   3rd Qu.:244.178
##  Max.   :20.200   Max.   :408.056
```

```
head(df)
```

```
##   time   mean y_min y_max       sd      var
## 1    0 4198.8  4195  4200 1.398412 1.955556
## 2    1 4198.4  4195  4200 1.429841 2.044444
## 3    2 4197.8  4195  4200 1.686548 2.844444
## 4    3 4196.7  4194  4199 1.702939 2.900000
## 5    4 4195.6  4194  4197 1.173788 1.377778
## 6    5 4194.8  4193  4197 1.229273 1.511111
```

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 against coefficient of variation (CV, in %):

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



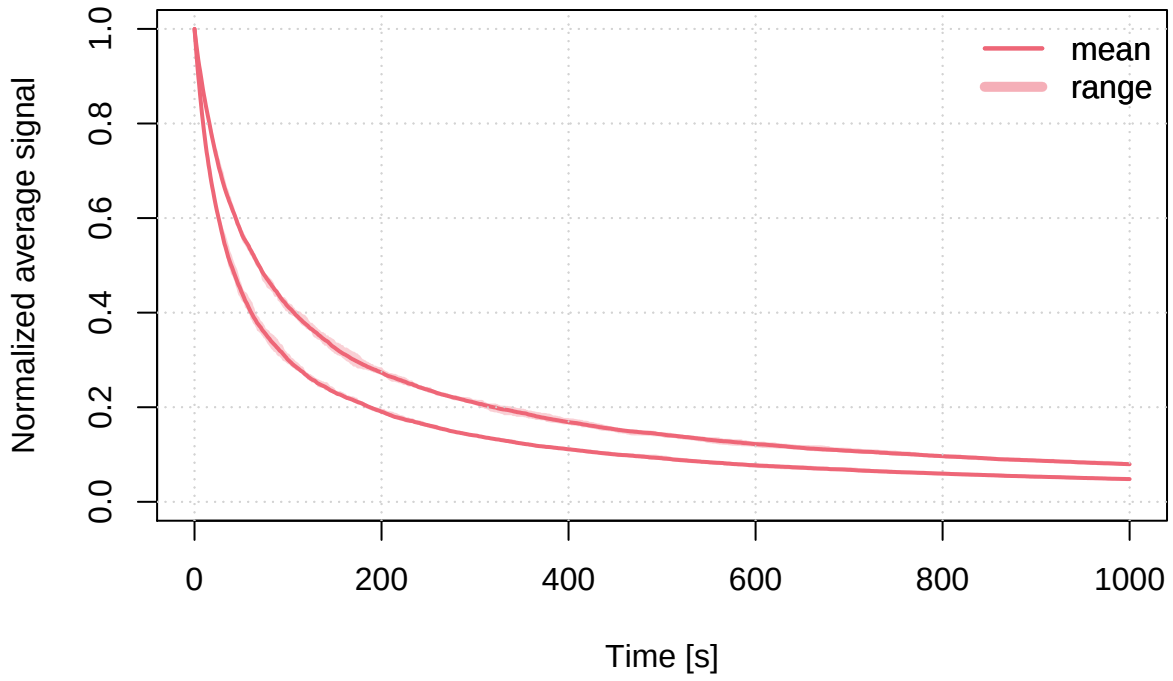
Example 2: Combining two plots

The following examples use again the tunneling model but for continuous wave (CW) infrared light stimulation (IRSL), and they combine two plots in one single plot window.

```
## set time vector
times <- seq(0, 1000)
```

```r
## Run MC simulation
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 and it will then iterate automatically over the results to create a combined plot.

```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) # here time = temperature
results <- lapply(r_c, function(x) {
  run_MC_TL_TUN(
    s = s,
    E = E,
    rho = rho,
    r_c = x,
    times = times
  )

})
```

The plot output can be highly customised to provide a better visual experience, e.g., the manual setting of the colours and the legend.

```r
## plot curves, but without legend
plot_RLumCarlo(
  object = results,
  ylab = "normalised TL signal",
  xlab = "Temperature [\u00b0C]",
  plot_uncertainty = "range",
  col = khroma::colour("bright")(length(r_c)),
  legend = FALSE,
  norm = TRUE
)

## add legend manually
legend(
  "topright",
  bty = "n",
  legend = paste0("r_c: ", r_c),
  lty = 1,
  col = khroma::colour("bright")(length(r_c))
)
```