PRIFYSGOL ABERYSTWYTH UNIVERSITY

Dr Sebastian Kreutzer

Adran Ddaearyddiaeth a
Gwyddorau Daear
Prifysgol Aberystwyth
Penglais, Aberystwyth, Ceredigion
Cymru, DU SY23 3DB

Swyddfa: F8
Ffôn: +44 (0) 1970 622658
E-bost: sebastian.kreutzer@aber.ac.uk
Gwefan: www.aber.ac.uk/cy/dges

Dr Sebastian Kreutzer

Department of Geography and
Earth Sciences
Aberystwyth University
Penglais, Aberystwyth, Ceredigion
Wales, UK SY23 3DB

Room: F8
Phone: +44 (0) 1970 622658
Email: sebastian.kreutzer@aber.ac.uk
Website: www.aber.ac.uk/en/dges

R Journal
Executive Editor
Prof Diana Cook

Subject: Add-on package: Motivation letter article re-submission
Manuscript reference: 2020-124

Dear Prof Cook,

Thank you for your feedback and for reconsidering our manuscript for publication in the *R Journal*.

We enclosed the revised version our manuscript

"RLumCarlo: Simulating Cold Light using Monte Carlo Methods"

by Sebastian Kreutzer, Johannes Friedrich, Vasilis Pagonis, Christian Laag, Ena Rajovic and Christoph Schmidt for consideration by the R Journal.

We carefully considered all suggestions and comments raised by the two reviewers and attached a detailed response to this letter (see following pages).
The reviewers flagged no scientific or major technical issues but made detailed suggestions to improve reading and structure of the manuscript tailoring it better to the readership of the *R Journal* (presumably) stemming from mathematics, statistics and computer science. Reviewer #2 found code-documentation mismatches we corrected with a new version of 'RLumCarlo' already on CRAN.

We hope that you will find our revised paper worth being considered for publication in the *R Journal*.

I am looking forward to your response! On behalf of the manuscript authors,

Your sincerely and Merry Christmas!

Sebastian Kreutzer

Yn unol â pholisi dwyieithog Prifysgol Aberystwyth, mae croeso i chi ohebu â'r Brifysgol yn Gymraeg neu yn Saesneg
In accordance with the bilingual policy of Aberystwyth University, you are welcome to correspond with the University in Welsh or in English

General response

We highly appreciate the thorough comments and suggestions voiced by the two reviewers. This manuscript is our first contribution prepared for the R Journal, and it was stimulating and helpful to receive views from outside of our bubble. For instance, intentionally, we kept some of the technical details related to the R implementation out of our manuscript. We believed that it might be boring to the readers because they have already a more profound knowledge of R but might want to learn more about the background of our implementation. On the other hand, we overlooked that readers may want to see a little more context.

To that end, we agree to almost all of the comments and suggestions raised by the reviewers. We revised our manuscript accordingly. In the following, we respond separately to each point.

Note: Unfortunately, the comments by reviewer #2 reached us two weeks after the comments by reviewer #1 and only a few hours away from the resubmission of the already heavily revised manuscript. Nevertheless, we did our best to give both reviews (and reviewers) the full attention they deserve. However, after we had already rewritten and restructured large parts of the text to follow the suggestions by reviewer #1, we kept further structural changes to a minimum.

Response to reviewer #1

> Article: The description of the work needs to be revised to help non-experts in the field (most readers of the R Journal) understand the problem and concepts better, while some technical details for experts from applied physics may be omitted. The article includes examples that show how to use the code, but also contains superfluous code blocks that should be omitted. A comparison with an alternative package in R is included, however, several other relevant packages mentioned in the cover letter are not mentioned in the article but should be commented on. Detailed recommendations are listed below.

We do agree. Supposing that the reviewer feels that our text does not read intelligible enough to most readers of the R Journal, indeed, there is room for improvements (we detail our changes further below).

The packages mentioned in the cover letter aimed at providing context to the editor allowing a first rough assessment of whether the manuscript might be at all suitable for the journal before sending it out for review. We did not mention those packages in the manuscript, because we felt that this would put the manuscript somewhat beyond its initial scope. Furthermore, since the corresponding author considerably contributed to half of the mentioned packages, we felt that too much self-appraisal might put off the readers. However, we now happily included this information but still tried to avoid the self-appraisal.

> Package: The package appears to be well written and documented, including a vignette showcasing the use beyond what is presented in the article. However, I have problems running the included example code on my machine, and get errors when running the simulation, see below.

We are sorry to read about these technical problems. We understand that nothing is more frustrating than a non-working code. Unfortunately, without further information on the system used by the reviewer, we can only guess the cause:

In summer 2020, the corresponding author encountered a very similar problem: https://github.com/rstudio/rstudio/issues/6692 (https://github.com/rstudio/rstudio/issues/6692)

This was caused by changes in R: https://developer.r-project.org/Blog/public/2020/03/17/socket-connections-update/index.html (https://developer.r-project.org/Blog/public/2020/03/17/socket-connections-update/index.html)

It appears to be, however, a particular *RStudio* problem for which workarounds exist. Additionally, and to ensure that we have not overlooked a severe bug, we added the code lines in question to our CI tests. At the same time, we updated RLumCarlo to support `'testthat >=` 3.0.0. We did not observe any error on the tested platforms (various Windows, Linux and macOS combinations for R-old to R-devel). The package has a test coverage of 100%, and every model has a short examples run also by CRAN. So far no error is flagged on the CRAN server farm. However, if the reviewer, regardless of the information provided above, still encounters the problem, we would need more details to reproduce the error and provide better support.

> Detailed comments:
>
> The abstract and first paragraph of the introduction are too technical, keeping in mind that this is a submission to the R Journal, where most readers are not familiar with the field of applied physics. In the abstract avoid discussing details about different modelling strategies, and instead focus on the presented package and the implementation therein.

We rewrote the abstract following the reviewer's advice. Now it reads more rigorously and does not anymore debate the different modelling strategies but the implementation in R.

> The opening paragraph of the introduction aims to place the work into context, but will be difficult to follow for most readers. Avoid reference to "see below" and the discussion of technical details here, and instead focus on the concept and broad setting of the work.

We revised the opening paragraph and greatly simplified the wording and also added a new introductory figure that may help to understand the idea of `'RLumCarlo'`.

> In the introduction it needs to be clear for outsiders what is actually being simulated, i.e. explain the physical phenomenon without use of technical language.

Similar to the abstract, we heavily revised the introduction (not completely rewritten though), and it is now greatly simplified. Contrary, the paragraph ‘cold light’, may now appear slightly redundant to the reviewer. However, to distinguish the processes we simulate from other phenomena a precise language is needed. We have to keep in mind that while the majority of the readers may not have a background in physics, other readers may find it somewhat disturbing that we approach such a topic without showing the necessary care.

> The authors refer to “birth-and-death” processes twice without explanation, these should be explained in the introduction.

We are thankful to the reviewer for flagging this. We had assumed that the concept of “birth-and-death” comes naturally to readers of the *R Journal* given their affinity to statistics. Beyond, we felt it would be sensible to mention for advanced readers that we are well aware of the similarities. Our simulations are Markov processes, however, with a transition allowed only in one direction (reduction of particles or ‘death process’).

But the reviewer is right, and the readership is too diverse. Hence we tried to make it more understandable with the rephrased introduction.

> The subsection on “cold light” can be improved by using diagrams when explaining the different processes (such as those given in Figure 1).

We added a new figure outlining the basic idea of `'RLumCarlo'` (now the first figure in the manuscript). Beyond that, we feel that additional graphics are not sensible and it would put the manuscript off track; drifting away from R and the simulation of luminescence with MC methods towards a general introduction to luminescence. For such an introduction, the referenced literature may be better suited.

> The final paragraph in the subsection is about modelling and thus should be moved to the next subsection on this subject.

We stripped this paragraph and now present it as a separate section, combined with the remainder of the paragraph from the introduction. This way it reads more consistent and allows the reader to follow the paragraph easily without notionally jumping back and forth.

> The article is on the implementation of the modular MC simulations, a discussion of particular models is out of scope, and hence the final paragraph on page 2 is superfluous and should be removed.

This paragraph is needed to put two aspects of our contribution into context: (1) energy-band luminescence models based on coupled differential equations and (2) `'RLumModel'`, the package we used to compare or validate, if you want to say so, our results. This mustn't come out of the blue at the end, because both approaches are conceptionally different. However, both use energy-band models. Therefore it is easy to mix them up.

Nevertheless, we did not ignore the reviewer's advice and merged this paragraph with other text on the conventional modelling in an own section.

> A number of R packages are used and mentioned, these should also be cited in the bibliography. You can use the R function citation("packagename") to obtain these references.

Thank you for flagging this. Our mistake and now corrected and cited as requested.

> The opening paragraph of the section "The concept of RLumCarlo" is confusing and should be more focused: the evolution of the conception is not relevant, instead give a clearer summary of the design as implemented. As mentioned this is the simplicity and flexibility provided by the modular setup for isolated effects that can be combined.

We rephrased the paragraph, and now it reads more focussed. Because we saw fit, we also clarified the ambiguity of the word 'clusters'; used multiple times in the text.

> The section "Implemented energy-band models" and Figure 1 describe the available models and the relevant parameters. However, the description is not clear for outsiders and needs to be explained better. This could be improved by using the diagrams in the introduction (as mentioned above) to fully explain the different processes. In addition, all letters used in the diagram (and their placement) need to be explained (R, A, r, r', rho are not mentioned in the text).

We extended the description and now mention the missing parameters in the text. Besides, as already mentioned in the text, more details are available in the package manual, the vignette and not at least in the cited literature. More information would render our already long manuscript too verbose.

> Before describing in detail one example implementation, the authors should give a conceptual overview that is abstracting the underlying iterative process over time, and what is happening at each iteration. This will help the reader understand the details in the following description.

Following the reviewers' advice, we reshuffled our text and moved the example algorithm for the radioactive decay further up and enhanced it through a detailed description.

> Some parameters are described a second time after Eq. (3). The common parameters explained before do not need to be repeated here, instead focus on those specific to the example only.

We now avoid the repetition of parameters.

> Section "The package design", first paragraph: the last three sentences should be summarised into one clearer sentence.

Rephrased as requested. Now it reads:

"RLumCarlo runs the simulations in virtual clusters on single or multicore systems using `'parallel'` (R Core Team, 2020), `'doParallel'` (Corporation and Weston, 2020) and `'foreach'` (Microsoft and Weston, 2020) supported by helper functions (Fig. 4) to summarise the results and to provide S3-class based graphical output."

> Section "Simple illustrative examples": the first code block should be separated, showing first the call for running the simulation and explaining the arguments better (How does the clusters argument relate to the theory discussed? Explanation of n_filled is not clear.), before showing how to generate the plot (and also explain the "main" argument for the call).

As advised, we separated the code blocks and better elaborated the function arguments. We refrained, however, to add too many details. The reader can find all those information more conveniently in the package manual (which will be always up-to-date). We also explained `main` (which is a standard argument from `graphics:plot.default` for the title).

> The printout of the output object (the list with the results) is not needed and should be removed.

Done.

> The following code block for generating Fig. 5(C) is also not needed, it is sufficient to specify how CV is computed.

We removed the code block and now detail the calculation of the coefficient of variation.

> Section “Advanced examples and further considerations”: the different uses of the name “cluster” is confusing, please change the names to make clear which type of clusters are being referred to (e.g. “MC cluster” when talking about a result from a single chain).

We amended our manuscript accordingly to distinguish between ‘MC clusters’ (no physical meaning) and ‘defect clusters’ (meaning concerning the simulated system). Although both amalgamate somewhat in `'RLumCarlo'`, depending on the perspective, which is wanted and needed.

> Section “Spatial correlation”: this section should be extended to explain how the mixing (as shown in Fig 6B) is implemented in the advanced mode of the code. In addition, more details about the clustering are needed: how is the cluster size selected for stats::cutree()? What type of linkage is used and why?

We admit that this is a weaker point in our manuscript and the implementation in `'RLumCarlo'`.

Even before we had been working on `'RLumCarlo'`, we sought an approach to simulate the spatial correlation of clusters. Unfortunately, this isn’t very easy from a physical point of view and thus has never really been accomplished. However, while working on `'RLumCarlo'`, we realised that such a correlation might be mimicked by adding meaning to the MC clusters through (so far dimensionless) coordinates to each group. However, there is still a lot of scientific legwork needed to explain real measured data. To that end, the choice of `stats::cutree()` is somewhat arbitrary, to allow any control of the cluster size.

We modified the text accordingly and now make clear that there is currently no real linkage between `stats::cutree()` and the physical process, except for control of the cluster size.

> Can you comment on why the full approach (Fig 6C) is more difficult and how it could be tackled in a future implementation?

The brief answer to that question reads: Just because it is technically possible in R (or any other programming language) it does not mean that it is physically meaningful. Our approach would easily allow an exchange of charger carriers (e.g., electrons), however, definition and test of suitable transfer functions (based on to be developed equations) are subject to future research projects.

> The description of Fig 6A is not fully clear: the models are spatially separated in the diagram, but position is irrelevant in the implementation?

Yes, the reviewer is right. The position has no relevance, and we clarified this in the text.

> Section “Comparison to RLumModel”: the code-blocks in this section are not needed and should be removed.

The code blocks account for the diversity of the readership. They are needed to set the physical parameters right. More importantly, the last code block includes a correction for an effect called “thermal quenching”; simplified: reduced light output with increasing temperature. While details and background are not of relevance to the reader, if not taken into account, the reader has no chance to reproduce our comparison of `'RLumModel'` and `'RLumCarlo'`.

We believe that the results in our contribution should render itself reproducible to be credible. Specialists often enough overlook the particular physical effect, thus we can impossibly expect that readers not familiar with our field know about it. Hence, we prefer to stick with the code blocks.

> Instead please discuss briefly the differences in interface.

We added two lines to explain that input parameters are optional in `'RLumModel'` and users provide a measurement sequence based on pre-defined models. This is the key difference (additional to the fundamentally different simulation approach, as outlined on various occasions in the text).

> Code comment: when running example code from the vignette or that included with the submission, I get the error messages of this type:

```
results <- run_MC_ISO_TUN(
  E = 1.2,
  s = 1e10,
  T = 200,
  N_e = 200,
  rho = 0.007,
  clusters = 10,
  times = seq(0, 5000)
  )
```

```
  Error in makePSOCKcluster(names = spec, ...) :
  Cluster setup failed. 7 of 7 workers failed to connect
```

Already addressed in the initial statement.

Response to reviewer #2

> First, I need to disclose that I do not know much about luminiscence and the physics behind it. Having said that, the authors have done a good job in explaining the phenomena and walk through some of the basics of the mathematics. I think the manuscript should be accepted with major revision.

We appreciate the honesty of the reviewer, and we are happy to read that our manuscript presents itself somewhat intelligible to non-experts of our field. This was the idea for submitting our contribution to the *R Journal*.

> The authors introduce a package, RLumCarlo, that provides several functions to simulate cold lights using Monte Carlo methods. From what I understand, this package is different from a related package, RLumModel, in that RLumModel simulates cold lights using deterministically. RLumCarlo is convenient: given a set of parameters, the functions simulate the luminescence signals over time (temperature) for multiple repeats. The package provides helpers functions that automatically aggregate the output of the multiple repeats, and plot the outputs (e.g., expectation and uncertainty). Currently the package seems to support only a few types of models, which may be a significant drawback for the package. Nevertheless, I agree with the authors that the package makes MC method accessible, especially to beginners.

We may comment on the 'significant drawback', because it is an understandable but perhaps unfortunate (for us) perception. There are two aspects to it: (1) Most relevant basic models including their allowed transition, are already part of `'RLumCarlo'`. (2) Unfortunately, there is no large pool of already available MC models for luminescence production. It does not mean that there are not more models available, but it needs time to develop and translate deterministic models into MC models. This is not always as easy as shown in the manuscript. In brief, more models are part of ongoing and future research.

> The article is generally well written. However, I struggle to understand some sections (see specific comments). I am particularly concerned about the "Spatial Correlation" section of the article. To me, the spatial correlation part of the package feels like it is trying to add some depth into the package, but it is unclear to me how readers can use this feature to understand more complex system.

It is not so much about understanding, this would be too much to ask of `'RLumCarlo'`, but an additional (new) way to simulate particular effects. A particular interpretation may follow later combined with new measurements (in the framework of, hopefully, funding projects).

In brief: In the past, luminescence simulation attempts made a couple of very convenient assumptions (see section "Towards Monte Carlo simulations"). One of those assumptions was that defects are distributed homogeneously in the dosimetric system (e.g., quartz crystal). However, we have no reason to believe that this has to be true in nature. Instead, it is highly likely that defects (e.g., in the form of an Al atom replacing Si in quartz) are clustered, i.e., spatially concentrated in a particular volume of the system (e.g., quartz crystal).

On the other hand, past simulations provided meaningful results. But this is the tricky part with models and simulations. They may appear to be ok, but we would not know whether we neglect a particular (critical) effect until we have tried to simulate it with another attempt which is more true to nature. Perhaps, we will

figure out that even with the spatial functionality, `'RLumCarlo'` will not instantaneously provide deeper insight, but this is subject to future research. Here, first of all, we enabled a feature to allow such a simulation (which was not possible before).

> It would be helpful that the authors state some potential uses for the system of clusters with spatial correlations. The transition into the “Spatial Correlation” section is drastic and I could not find a compelling reason why system of clusters is needed. And that there is no clear example in this section. It is also somewhat confusing that, “cluster” in the previous section can be interpreted as “repeats”, but in this section it is actually a member of a more complicated system. I do not think the brief discussion about clusters in “Advanced examples and further considerations” section addressed this conceptual change. Finally, since “cluster” is no longer a “repeat” in this section, what are ways to run multiple simulations for the cluster system?

The reviewer is right and we already extended and rephrased the relevant sections as detailed for reviewer #1.

Besides, the word cluster originates from the package `parallel` we use for the multicore processing. Different scientific communities use similar words but assign different meanings. Nevertheless, the word came in handy also to simulate separate MC process (in parallel or sequentially does not matter; independence is essential). A better word, perhaps, would be ‘MC chains’ then there would be no confusion with ‘dosimetric clusters’, which have a physical meaning. The problem with ‘MC chains’ (we now at least mention the potential analogy in the text) is that people working with Bayesian modelling (likely in the R community) might have very particular expectations on such MC chains and we did not want to engage in this discussion because it does not matter for our contribution.

Nevertheless, we hope that the reviewer will find our rephrased paragraphs better and easier to read.

> For the package, I find the code straightforward and easy to follow. However, I have encountered errors when running the sample code (in the article) for cluster system with spatial correlation.

We assume that the reviewer means the R code modified based on the examples provided in the manuscript and the reviewer saw something like:

```
Error in { : task 1 failed - "argument "A" is missing, with no default"
```

If the reviewer rans the package example for `run_MC_CW_IRSL_LOC()`

```
run_MC_CW_IRSL_LOC(
 A = 0.12,
 times = 0:100,
 clusters = 50,
 n_filled = 100,
 r = 1e-7,
 method = "seq",
 output = "signal"
)
```

but removing `A = 0.12`. We will elaborate the cause in the following answer. Besides, we tested all examples *as is* in the manuscript and found no errors (as replied to reviewer #1, package examples are also tested by CRAN without showing any error).

> Apparently, r and times argument had no default. Going through the reference manual, I found out that several functions had similar problems. Although the reference manual claims that r and times in most of the run_MC_*() functions are “with default”, they were actually without default values, resulting in errors.

We are thankful to the reviewer for spotting this. The following functions had a documentation/code mismatch (which is now corrected in `'RLumCarlo'` v0.1.7 already released on CRAN):

`run_MC_CW_IRSL_LOC()`, `run_MC_CW_IRSL_TUN()`, `run_MC_CW_OSL_DELOC()`, `run_MC_ISO_DELOC()`, `run_MC_ISO_LOC()`, `run_MC_ISO_TUN()`, `run_MC_LM_OSL_DELOC()`, `run_MC_LM_OSL_LOC()`, `run_MC_LM_OSL_TUN()`, `run_MC_TL_DELOC()`, `run_MC_TL_LOC()`, `run_MC_TL_TUN()`

In each function, up to two arguments claimed default values where we required an input instead. We may elaborate the cause for this human error: In each function, we provide a documentation scheme such as:

`<param>``<type>``<required,default,optional>`

This is a documentation scheme we used to make it easier for the user. Such a schema is possible with the R documentation system (and `roxygen2`), but not actively supported. Means, there is no cross-check between the R function definition and its documentation of whether a parameter has a default value or not. In our case, we first had default parameters. Still, we later changed it back to ‘required’, and we had overlooked to update the documentation. We apologize for the trouble we have caused.

> Additionally, I find it difficult to understand the h argument in the create_ClusterSystem() function. I know that it is the height threshold in the stats::cutree() function but how would a person using create_ClusterSystem() knows what h to choose? Is there an intuitive explanation for it? I would imagine myself wanting to specify the number of cluster group instead of a threshold for the heights (which I cannot visualize the scale and variability).

The reviewer is right, and this was also flagged by reviewer #1. For the moment, it does not matter, and the `h` value is just one value to allow playing with the parameters (see also comments to reviewer #1).

> The following section is my specific comments. Specific comments Introduction: “Such a presentation was beyond the scope of previous articles, …” I do not understand what are the “previous articles” here and in general I am confused by the sentence.

Thank you for spotting this. Meant were our previous articles published in the *Journal of Luminescence*. We added the missing references.

> Paragraph 2 of Towards Monte Carlo simulations: Kulkarni (1994) also reported a “statistical fluctuation” Why quote unquote statistical fluctuation? Would it be helpful to explain this feature (or problem) in a few more words? E.g., that MC provides different output for each simulation run.

It was meant as a direct quote referring to Kulkarni (1994). Still, we forgot to add the page number, which would have made it easier for reader to identify the quote as an actual (direct) quote. What Kulkarni (1994) meant was nothing more than the noise, like scatter he observed due to the stochastic process of the simulation. A “fluctuation”, which was not wanted back in the days. We added the missing page number and clarified what Kulkarni meant.

> Figure 1 caption: “Site note: …” Side note?

Thank you, corrected.

> The concept of RLumCarlo: First paragraph I have a hard time reading this paragraph. I think the authors want to draw distinction between RLumModel and RLumCarlo here. But as someone who has no knowledge about RLumModel, I struggle with this paragraph. Could this be rewritten to state clearly what RLumModel does, and why RLumCarlo can do something that RLumModel cannot?

We revised this part following the suggestions by reviewer #1, and we hope that it now reads more intelligible, pointing out that the ‘sole’ common ground of `'RLumModel'` and `'RLumCarlo'` is the approach to use energy-bands models to simulate luminescence production in natural minerals using R. Beyond, `'RLumModel'` uses coupled-differential equations and `'RLumCarlo'` difference equations, used in MC simulations. Both approaches are fundamentally different.

> Implementation example for the OTOR model: “For TL and ISO applying the localised or delocalised model p(t) is …” Why are TL and ISO here “coded” (different font indicating the two are part of R code)?

`TL` and `ISO` are indeed the abbreviations used in the R code as part of the function names. This was obviously not as straightforward to understand as we had hopped. Now it reads:

“For TL (functions named `run_MC_TL_<model>()`) and isothermal (functions named `run_MC_ISO_<model>()`) applying the localised or delocalised model $p(t)$ becomes …”

> Implementation example for the OTOR model: Nested loop code “for (j in 1:max(n)) { … }” n in this code chunk is a numeric vector with length of 1. Does not make sense to use “max(n)” here; not wrong, but can be confusing.

Agreed, and our apology. It was a left-over from a more complicated example where `n` was a vector.

> In the next line of code “if (runif(1) < P && n > 0)”, the use of && is again not wrong, but confusing since it is more common for R users to stick to using & instead of &&.

We stick with the `&&`, because `&&` and `&` do not show the same behaviour. Quoting from the R manual (`help("&&")`):

The shorter form performs element wise comparisons in much the same way as arithmetic operators. The longer form evaluates left to right examining only the first element of each vector. […] The longer form is appropriate for programming control-flow and typically preferred in if clauses.

> Furthermore, the nested for loops in R seems unnecessary. Specifically, the for (j in 1:n) part can be vectorised: e.g., sum(runif(n) < P) gives the number of electron to be removed at loop t. One can check if n > 0 at the start of loop t before determining the number of electron to be removed too. I understand that the authors may have implemented the nested for loop in C++, which would be appropriate, and use the analogous R code here for illustration purpose.

Agreed, perhaps this was too confusing. We added:

Below we used R code for illustrative reasons, while the package implementation is written in C++.

> The package design: “While the apparent reason for using C++ was speed, the implementation could have been programmed more efficiently. However, we wanted to allow code inspection by non-specialists from our field, who may wish to implement other models alike.” I am confused about “the implementation could have been programmed more efficiently” here. Are the authors saying that they could have not used C++, and program their MC algorithm more efficiently in R? Or that their C++ implementation is not efficient? I also struggle to relate to the following sentence: wouldn’t non-specialists have better chance understanding R code than C++?

As Martyn Plummer (e.g., R Core Team, `JAGS`, `rjags`) once wrote in his blog: “You can always make it faster …” (https://martynplummer.wordpress.com/2016/09/14/you-can-always-make-it-faster/). Our statement is the forestalled answer to “Why did write one function for each model-stimulation mode combination. Why not using one function for each stimulation mode and then select the appropriate model?”

Experience has taught that more advanced users tend to make a lot of well-meant suggestions refactoring the code; particularly when it comes down to C++ code. However, if we would have aimed at a super fast and super efficient implementation, we would have used C instead of C++ interfaced through `'Rcpp'`. Our design is a compromise, reasonably fast and still not overly complicated.

Pure R was not faster. We tried, of course, vectorised; still, the overhead from the repeated parsing put a heavy load on the simulation for large numbers.

We could have also condensed the modelling core into one neat C++ function, but this renders the code not reader-friendly. The current solution allows, e.g., other colleagues from our field, to duplicate one model-stimulation mode combination and add their ideas, without considering all different model and stimulation modes. And the broader R community gets an idea.

This explanation would be too long for the manuscript, therefore the paragraph flagged by the reviewer. Besides, we replaced the word ‘efficiently’ by ‘concisely’

> Paragraph 2 of The package design: “As indicated above, …” I think the authors refer to the basic implementation algorithm, it would be better to be specific here.

Thank you, now we make this clear as requested.

> Paragraph 6 of Comparison to RLumModel: “N_e was dived by” Divided by?

Corrected. Thank you for spotting this, the typo was still in the manuscript; unbelievable even after all the careful reading.