Re: TUM T38 MD Tutorial for the Living Journal of Computational Molecular Science

Mala L Radhakrishnan <mradhakr@wellesley.edu>

Wed 10/16/2024 12:49 PM

To:Luis Vollmers <luis.vollmers@tum.de>;

Cc:Martin Zacharias <zacharias@tum.de>;

Dear Luis,

Apologies again about the delay. Thanks for your presubmission letter inquiry regarding your tutorial/ training article on MD simulations that takes a course-like approach.   Though this might be different in tone from other articles we publish, we think it would be useful for many students getting started in coursework or research at both the undergraduate or graduate levels.   Please consider this our formal acceptance of your pre-submission letter (noting, of course, that this does not guarantee acceptance of the ultimately submitted tutorial).

We do want to remind you that, given the length of your manuscript and the number of activities, the timeline for reviewing will be rather long (I think you had said you were ok with that).

We look forward to receiving your submission. You technically have 6 months, but it looks like you may be ready to submit sooner than that. Please let us know if you have any questions as you prepare your manuscript.

Thanks,

Mala

On Tue, Sep 24, 2024 at 7:44 AM Luis Vollmers <luis.vollmers@tum.de> wrote:

> Dear Mala,
>
> Attached is the pre-submission letter to the previously discussed tutorial/training article hybrid.
>
> I am looking forward to your reply.
>
> Sincerely,
>
> Luis Vollmers
>
> ---
>
> **From:** Mala L Radhakrishnan <mradhakr@wellesley.edu>
> **Sent:** Monday, May 20, 2024 4:30:15 AM
> **To:** Luis Vollmers
> **Cc:** tutorials@livecomsjournal.org; Martin Zacharias; Maria Reif; Managing Editors
> **Subject:** Re: TUM T38 MD Tutorial for the Living Journal of Computational Molecular Science

Hi Luis,

Thanks -- looking forward to seeing your presubmission letter which addresses how your tutorial complements and uniquely contributes to specific learning goals beyond the existing LiveCoMS tutorials. In addition to describing a system and communicating results, like your attached exercises do, please make sure to clearly articulate the learning goals/objectives of your tutorial, so we can easily assess what readers are supposed to walk away with after going through the tutorial. Thanks!

Mala

On Tue, May 7, 2024 at 2:59 PM Luis Vollmers <luis.vollmers@tum.de> wrote:

> Dear Mala,
>
> Thank you very much for your very detailed answer. I will start to compile a presubmission letter as soon as possible.
>
> Following your recommendation, I will include an extensive discussion of available MD simulation tutorials as part of the presubmission letter.
>
> The multi-group collaborative effort also sounds very tempting; however, it seems to be a bit out of scope in the current situation. Nevertheless, I will discuss this option with my peers and may come back to you on that topic.
>
> Materials are currently saved in a private GitLab repository, but with the presubmission letter, I will move them into a public GitHub repository. I have attached the materials necessary for Exercise 2 as a zip archive for your review. The archive contains two directories: 'student' and 'teacher.' The 'student' directory includes the input files necessary to complete the tasks, and the 'teacher' directory contains solutions, which typically consist of the input files found in the 'student' directory along with a Bash script that runs the simulations and analyzes the trajectories as needed. The 'teacher' directory also includes a 'model report' to demonstrate what the results should look like.
>
> The extended timeframe sounds very reasonable.
>
> I am looking forward to continuing the conversation with you.
>
> All the best,
>
> Luis
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> ---
>
> **From:** Mala L Radhakrishnan <mradhakr@wellesley.edu>
> **Sent:** Monday, May 6, 2024 5:01 PM

To: Luis Vollmers
Cc: tutorials@livecomsjournal.org; Martin Zacharias; Maria Reif; Managing Editors
Subject: Re: TUM T38 MD Tutorial for the Living Journal of Computational Molecular Science

Dear Luis,

Thank you for reaching out. We do think that there continues to be a need for tutorials that provide validated and robust practices in MD simulation, so this could be a potentially useful contribution. The first thing to do to continue the process would be for you to draft a formal presubmission letter - (details are found if you scroll down this page.)

One important thing to address in your letter is how this work complements/augments existing LiveCoMS tutorials and best practices articles (and potentially our other categories also) -- we have published multiple tutorials on various aspects of MD simulations, including ones on general ways to "get started" and carry out best practices as well as those specific to certain software packages. Explicitly placing your work within the context of these existing tutorials and other article types would be great -- and perhaps focusing your tutorial on aspects that might be lacking in the existing tutorial space -- particularly those for which your group might have unique expertise -- and articulating that would be terrific. A more general, high-level, and broad article on MD might also be appropriate, but then it might be useful to have a multi-group collaboratory effort toward creating such a document -- and depending on the scope, that's something we can perhaps help catalyze if there is interest in that.

Your attachment includes some interesting examples and applications -- it might also be useful to point us to the course materials you mention if those are available on line as well.

I don't think the length is hugely problematic, especially if it helps the pedagogical value of the tutorial, although you might be able to shorten it if you do find overlaps between what you present and what is available in our existing best practices and tutorials. It might understandably take us longer to have a longer paper go through the review process because finding people to review tutorials is already difficult due to the fact that we ask them to work through the tutorials. But so long as you are ok with the timeframe, this length is ok for us so long as it's warranted.

Hope this helps, and looking forward to continuing the conversation with you. Please let me know if you have any questions as you put together your presubmission letter!

Mala

On Wed, Apr 24, 2024 at 1:15 PM Luis Vollmers <luis.vollmers@tum.de> wrote:
> Dear Dr. Mala Radhakrishnan,
>
> My name is Luis Vollmers, and I am a PhD candidate at the Technical University of Munich. I am writing to inquire about the possibility of submitting a detailed tutorial draft to LiveCOMS.
>
> With a total of 53 pages, I noticed that our tutorial contains significantly more pages than usual for LiveCOMS. Would such an extensive tutorial nevertheless be considered for submission to LiveCOMS? Should there be interest from your editorial team, I am fully prepared to undertake significant refinement and to align it with LiveCOMS' editorial standards, since the draft is currently in a preliminary state just for showcasing (see attachment).
>
> The tutorial's working title is: 'From Physical Principles to Drug Discovery - Understanding Molecular Dynamics Simulations and Molecular Modeling'. It aims not only to teach specific software functionality but especially stands out by educating users on how to understand molecular dynamics and access simulation results qualitatively. This is facilitated through a programmatic approach and by relating simulation data to physical principles. It originates from a Biophysics Master's course, with downloadable files, solutions, and templates already

in place.

There are many different software packages involved, all of them open source (e.g., GROMACS, Python, AutoDock, Grace, AmberTools, etc.).

I would appreciate it if you could let me know whether such a tutorial is of interest to your editorial board.

I am looking forward to hearing from you.

Sincerely,

Luis Vollmers