

This is the title [Article v1.3]

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Abstract This particular document provides a skeleton illustrating key sections for a Training article. Please see the sample `sample-document.tex` in github.com/livecomsjournal/article_templates/templates for additional information on and examples of using the LiveCoMS LaTeX class. Here we also assume familiarity with LaTeX and knowledge of how to include figures, tables, etc.; if you want examples, see the sample just referenced.

In your work, in this particular slot, please provide an abstract of no more than 250 words. Your abstract should explain the main contributions of your article, and should not contain any material that is not included in the main text. Please note that your abstract, plus the authorship material following it, must not extend beyond the title page or modifications to the LaTeX class will likely be needed.

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1 Introduction

Here you would explain what problem you are tackling and briefly motivate your work.

In this particular template, we have removed most of the usage examples which occur in `sample-document.tex` to provide a minimal template you can modify; however, we retain a couple of examples illustrating more unusual features of our templates/article class, such as the checklists, and information on algorithms and pseudocode.

Keep in mind, as you prepare your manuscript, that you should plan for a representative image which will be used to highlight your article on the journal website and publications. Usually, this would be one of your figures, but it must also be uploaded separately upon article submission. We give specific guidelines for this image on the journal website in the section on article submission (see <https://livecomsjournal.github.io/authors/policies/index.html#article-submission>).

[github.io/authors/policies/index.html#article-submission](https://livecomsjournal.github.io/authors/policies/index.html#article-submission)).

Additionally, for well-formatted manuscripts, we recommend that you let LaTeX handle figure/table placement for you as much as possible, so please avoid specifying strenuous float instructions like '[h!]' and '[H]' as much as possible.

1.1 Scope

Training articles are largely self-contained and introduce readers to the theory and/or typical procedures for a particular aspect of molecular simulation.

Training articles need not refer to specific software commands and procedures but may do so to further the pedagogical goals of the paper.

As needed, training articles are likely to display more details of calculations than typically are shown in research articles, for example, noting any mathematical principles or

“tricks” used to derive key results.

The scope of the training article should be clearly defined. This will often happen in a specific section or subsection in the article itself.

2 Prerequisites

Training articles should clearly state the target audience and knowledge prerequisites. Key prerequisites should be noted in the article abstract to permit readers to rapidly ascertain an articles suitability.

2.1 Background knowledge

Although the authors may imagine a particular career-level (e.g., undergraduate or graduate), given the diversity of disciplinary curricula, it is more important to specify precisely any knowledge prerequisites (e.g., vector calculus, basic thermodynamics).

2.2 Software/system requirements

If a particular software or programming environment plays a central role in the article, that should be specified.

3 Content and links

A training article may on additional files and materials; clearly indicate where and how these are available, with links, and how they are being archived for the long-term and maintained so they stay current. You will likely want to reference your GitHub repository as a central point to access all of this information, and then the GitHub repository may link out to other content as needed.

4 Checklists

Training articles do not necessarily require the use of a checklist as in Best Practices documents; however, they can include these if desired. Several useful checklist formats are available, with examples presented in `sample-document.tex` in github.com/livecomsjournal/article_templates/templates. One example is shown here.

5 Author Contributions

(Explain the contributions of the different authors here)

For a more detailed description of author contributions, see the GitHub issue tracking and changelog at <https://github.com/myaccount/homegithubrepository>.

6 Other Contributions

(Explain the contributions of any non-author contributors here) For a more detailed description of contributions from the community and others, see

A LIST

Single-column checklists are also straightforward by removing the asterisk

- ☐ First thing let's do an item which breaks across lines to see how that looks
- ☐ Also remember
- ☐ And finally

ANOTHER LIST

This is some further description.

- ☐ First thing
- ☐ Also remember
- ☐ And finally

the GitHub issue tracking and changelog at <https://github.com/myaccount/homegithubrepository>.

7 Potentially Conflicting Interests

Declare any potentially conflicting interests here, whether or not they pose an actual conflict in your view.

8 Funding Information

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