

This is the title : v1.3

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Abstract This particular document provides a skeleton illustrating key sections for a Best Practices document. 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.

2 Prerequisites

Here you would identify prerequisites/background knowledge that are assumed by your work and your checklist which you view as critical, ideally giving links to good sources on these topics. Checklists are normally focused on errors made by

users with training and experience in molecular simulations, so you can assume a basic familiarity with the fundamentals of molecular simulations.

3 Checklist

Here we use a full-page checklist with multiple sections, so it will appear on a separate page of the sample PDF. Other checklist formats are possible, as shown in the sample `sample-document` in github.com/livecomsjournal/article_templates/templates.

Your checklist should include a succinct list of steps that people should follow when carrying out the task in question. This is provided to ensure certain basic standards are followed and common but critical major errors are avoided. Note that a checklist is not intended to cover *all* important steps, but rather focus on the most common reasons for failure or

incorrect results, or issues which are particularly crucial.

4 Rationale

Your Rationale section, or sections, can follow or precede your checklist (we expect that often, following the checklist will be preferable) and provide the necessary rationale for the checklist, and act as more complete *best practices* description. This should include 1) significant detail as to the possible alternative ways to accomplish a given task, 2) description of advantages and disadvantages of the various approaches, and 3) significant literature documentation about reasons for choices.

4.1 Algorithms and Pseudocode

The `algpseudocode` and `algorithms` packages is loaded by the document class. **Algorithm 1** was taken directly from the package documentation. (Please do not load `algorithm2e`; it's not compatible with `algpseudocode` nor `algorithms`!)

Algorithm 1. Euclid's algorithm

```

procedure EUCLID( $a, b$ )           ▷ The g.c.d. of  $a$  and  $b$ 
   $r \leftarrow a \bmod b$ 
  while  $r \neq 0$  do               ▷ We have the answer if  $r$  is 0
     $a \leftarrow b$ 
     $b \leftarrow r$ 
     $r \leftarrow a \bmod b$ 
  end while
  return  $b$                        ▷ The gcd is  $b$ 
end procedure

```

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 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

FMS acknowledges the support of NSF grant CHE-1111111.

FIRST LIST

You can easily make full width checklists that take a whole page

- ☐ Items in your checklist can and should reference sections where the cited issues are discussed in detail, such as Section 4.1
- ☐ Also remember
- ☐ And finally

SECOND LIST

This is some further description.

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

THIRD LIST

This is some further description.

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

FOURTH LIST

This is some further description.

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