# This is the title [Article v1.3]

Firstname Middlename Surname<sup>1\*</sup>, Firstname Middlename Familyname<sup>1,2†§</sup>, Firstname Initials Surname<sup>2†¶</sup>, Firstname Surname<sup>2\*</sup>

<sup>1</sup>Institution 1; <sup>2</sup>Institution 2

This LiveCoMS document is maintained online on GitHub at https:

to provide feedback, suggestions, or help improve it, please visit the GitHub repository and participate via the issue tracker

This version dated September 21, 2019

**Abstract** This particular document provides a skeleton illustrating key sections for a Computational Comparisons document. Please see the sample sample-document.tex in //github.com/myaccount/homegithub.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.

#### \*For correspondence:

email1@example.com (FMS); email2@example.com (FS)

Present address: §Department, Institute, Country; ¶Department, Institute, Country

#### Introduction

Here you would explain what problem you are tackling and briefly motivate your work; why is a comparison needed here? What do the tools you are comparing do?

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 but we retain an example on algorithms and pseudocode.

# Methodology

Here (and in other sections if needed) you would describe how you compared the software in question, with subsections as needed. Perhaps you may also need to comment here on why you did not include certain pieces of software or how these might be included in the future.

## 2.1 Physical systems and properties

What did you calculate, on what systems? Why did you make that choice?

#### 2.2 Methodology for comparison

How did you compute what you're comparing? What software versions did you use? How would the software be accessed?

#### 2.2.1 Method selection

How did you select which protocols to use? How are you certain these are representative? Would a naive user get similar performance?

#### 2.2.2 Supporting files

Are there run scripts or files others would need to reproduce your work? Are these provided in your GitHub repo, or how

<sup>&</sup>lt;sup>†</sup>These authors contributed equally to this work

<sup>&</sup>lt;sup>‡</sup>These authors also contributed equally to this work

would they be accessed? How exactly would someone reproduce/extend this work?

#### 2.2.3 Error analysis

You may wish to devote particular attention to error analysis.

#### 3 Results

You would give results.

#### 4 Discussion and conclusions

You may perhaps wish to revisit the issue of what performance a naive user might expect, 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 <a href="https://github.com/myaccount/homegithubrepository">https://github.com/myaccount/homegithubrepository</a>.

### **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.

# **Author Information** ORCID:

Author 1 name: AAAA-BBBB-CCCC-DDDD Author 2 name: EEEE-FFFF-GGGG-HHHH

# References