

¹ **Formatting Open Science: agilely creating
multiple document formats for academic
manuscripts with Pandoc Scholar**

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¹⁰ **ABSTRACT**

The timely publication of scientific results is essential for dynamic advances in science. The ubiquitous availability of computers which are connected to a global network made the rapid and low-cost distribution of information through electronic channels possible. New concepts, such as Open Access publishing and preprint servers are currently changing the traditional print media business towards a community-driven peer production. However, the cost of scientific literature generation, which is either charged to readers, authors or sponsors, is still high. The main active participants in the authoring and evaluation of scientific manuscripts are volunteers, and the cost for online publishing infrastructure is close to negligible. A major time and cost factor is the formatting of manuscripts in the production stage. In this article we demonstrate the feasibility of writing scientific manuscripts in plain markdown (MD) text files, which can be easily converted into common publication formats, such as PDF, HTML or EPUB, using pandoc. The simple syntax of markdown assures the long-term readability of raw files and the development of software and workflows. We show the implementation of typical elements of scientific manuscripts – formulas, tables, code blocks and citations – and present tools for editing, collaborative writing and version control. We give an example on how to prepare a manuscript with distinct output formats, a DOCX file for submission to a journal, and a LATEX/PDF version for deposition as a PeerJ preprint. Further, we implemented new features for supporting ‘semantic web’ applications, such as the ‘journal article tag suite’ - JATS, and the ‘citation typing ontology’ - CiTO standard. Reducing the work spent on manuscript formatting translates directly to time and cost savings for writers, publishers, readers and sponsors. Therefore, the adoption of the MD format contributes to the agile production of open science literature. Pandoc Scholar is freely available from <https://github.com/pandoc-scholar>.

¹¹ **Keywords:** open science, document formats, markdown, latex, publishing, typesetting

12 **INTRODUCTION**

13 Agile development of science depends on the continuous exchange of information between researchers
14 (Woelfle, Olliaro & Todd, 2011). In the past, physical copies of scientific works had to be produced and
15 distributed. Therefore, publishers needed to invest considerable resources for typesetting and printing.
16 Since the journals were mainly financed by their subscribers, their editors not only had to decide on the
17 scientific quality of a submitted manuscript, but also on the potential interest to their readers. The avail-
18 ability of globally connected computers enabled the rapid exchange of information at low cost. Yochai
19 Benkler (2006) predicts important changes in the information production economy, which are based on
20 three observations:

- 21 1. A nonmarket motivation in areas such as education, arts, science, politics and theology.
- 22 2. The actual rise of nonmarket production, made possible through networked individuals and coor-
23 dinate effects.
- 24 3. The emergence of large-scale peer production, e.g. of software and encyclopedias.

25 Immaterial goods such as knowledge and culture are not lost when consumed or shared – they are ‘non-
26 rival’ –, and they enable a networked information economy, which is not commercially driven (Benkler,
27 2006).

28 **Preprints and e-prints**

29 In some areas of science a preprint culture, i.e. a paper-based exchange system of research ideas and
30 results, already existed when Paul Ginsparg in 1991 initiated a server for the distribution of electronic
31 preprints – ‘e-prints’ – about high-energy particle theory at the Los Alamos National Laboratory (LANL),
32 USA (Ginsparg, 1994). Later, the LANL server moved with Ginsparg to Cornell University, USA, and
33 was renamed as arXiv (Butler, 2001). Currently, arXiv (<https://arxiv.org/>) publishes e-prints re-
34 lated to physics, mathematics, computer science, quantitative biology, quantitative finance and statistics.
35 Just a few years after the start of the first preprint servers, their important contribution to scientific com-
36 munication was evident (Ginsparg, 1994; Youngen, 1998; Brown, 2001). In 2014, arXiv reached the
37 impressive number of 1 million e-prints (Van Noorden, 2014).

38 In more conservative areas, such as chemistry and biology, accepting the publishing prior peer-review
39 took more time (Brown, 2003). A preprint server for life sciences (<http://biorxiv.org/>) was
40 launched by the Cold Spring Harbor Laboratory, USA, in 2013 (Callaway, 2013). *PeerJ preprints*
41 (<https://peerj.com/preprints/>), started in the same year, accepts manuscripts from biological
42 sciences, medical sciences, health sciences and computer sciences.

43 The terms ‘preprints’ and ‘e-prints’ are used synonymously, since the physical distribution of preprints
44 has become obsolete. A major drawback of preprint publishing are the sometimes restrictive policies of
45 scientific publishers. The SHERPA/RoMEO project informs about copyright policies and self-archiving
46 options of individual publishers (<http://www.sherpa.ac.uk/romeo/>).

47 **Open Access**

48 The term ‘*Open Access*’ (OA) was introduced 2002 by the Budapest Open Access Initiative and was
49 defined as:

50 “*Barrier-free access to online works and other resources. OA literature is digital, online, free of charge*
51 (*gratis OA*), and free of needless copyright and licensing restrictions (*libre OA*).” (Suber, 2012)

52 Frustrated by the difficulty to access even digitized scientific literature, three scientists founded the *Public*
53 *Library of Science (PLoS)*. In 2003, *PLoS Biology* was published as the first fully Open Access journal
54 for biology (Brown, Eisen & Varmus, 2003; Eisen, 2003).

55 Thanks to the great success of OA publishing, many conventional print publishers now offer a so-called
56 ‘Open Access option’, i.e. to make accepted articles free to read for an additional payment by the authors.
57 The copyright in these hybrid models might remain with the publisher, whilst fully OA usually provide

58 a liberal license, such as the Creative Commons Attribution 4.0 International (CC BY 4.0, <https://creativecommons.org/licenses/by/4.0/>).

60 OA literature is only one component of a more general *open* philosophy, which also includes the access
61 to scholarships, software, and data (Willinsky, 2005). Interestingly, there are several different ‘schools
62 of thought’ on how to understand and define *Open Science*, as well the position that any science is open
63 by definition, because of its objective to make generated knowledge public (Fecher & Friesike, 2014).

64 **Cost of journal article production**

65 In a recent study, the article processing charges (APCs) for research intensive universities in the USA
66 and Canada were estimated to be about 1,800 USD for fully OA journals and 3,000 USD for hybrid
67 OA journals (Solomon & Björk, 2016). PeerJ (<https://peerj.com/>), an OA journal for biological
68 and computer sciences launched in 2013, drastically reduced the publishing cost, offering its members a
69 life-time publishing plan for a small registration fee (Van Noorden, 2012); alternatively the authors can
70 choose to pay an APC of 1,095 USD, which may be cheaper, if multiple co-authors participate.

71 Examples such as the *Journal of Statistical Software* (JSS, <https://www.jstatsoft.org/>) and *eLife*
72 (<https://elifesciences.org/>) demonstrate the possibility of completely community-supported OA
73 publications. **Fig. 1** compares the APCs of different OA publishing business models.

74 *JSS* and *eLife* are peer-reviewed and indexed by Thomson Reuters. Both journals are located in the
75 Q1 quality quartile in all their registered subject categories of the Scimago Journal & Country Rank
76 (<http://www.scimagojr.com/>), demonstrating that high-quality publications can be produced without
77 charging the scientific authors or readers.

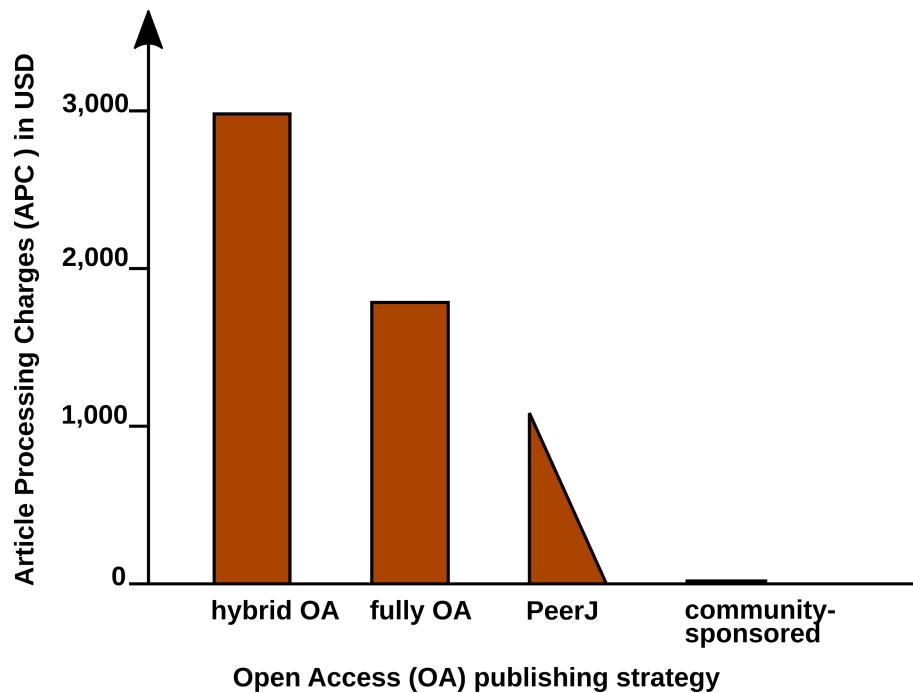


Figure 1. Article Processing Charge (APCs) that authors have to pay for with different Open Access (OA) publishing models. Data from (Solomon & Björk, 2016) and journal web-pages.

78 In 2009, a study was carried out concerning the “*Economic Implications of Alternative Scholarly Publishing Models*”, which demonstrates an overall societal benefit by using OA publishing model (Houghton
79 et al., 2009). In the same report, the real publication costs are evaluated. The relative costs of an article
80 for the publisher are represented in **Fig. 2**.

82 Conventional publishers justify their high subscription or APC prices with the added value, e.g. journalism
83 (stated in the graphics as ‘non-article processing’). But also stakeholder profits, which could be as

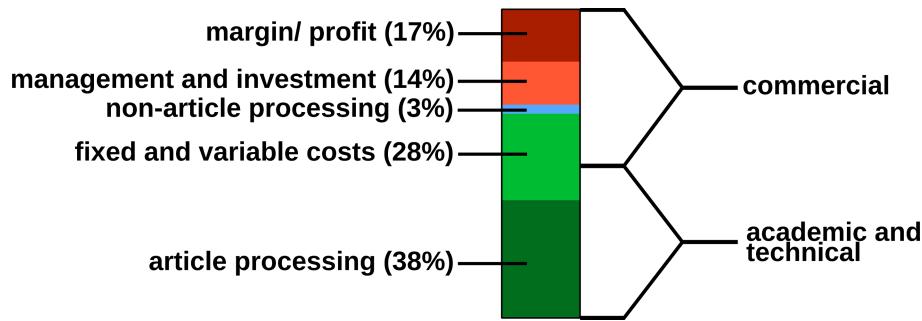


Figure 2. Estimated publishing cost for a ‘hybrid’ journal (conventional with Open Access option). Data from (Houghton et al., 2009).

84 high as 50%, must be considered, and are withdrawn from the science budget (Van Noorden, 2013).
 85 Generally, the production costs of an article could be roughly divided into commercial and academic/
 86 technical costs (Fig. 2). For nonmarket production, the commercial costs such as margins/ profits, man-
 87 agement etc. can be drastically reduced. Hardware and services for hosting an editorial system, such as
 88 Open Journal Systems of the Public Knowledge Project (<https://pkp.sfu.ca/ojs/>) can be provided
 89 by public institutions. Employed scholars can perform editor and reviewer activities without additional
 90 cost for the journals. Nevertheless, ‘article processing’, which includes the manuscript handling during
 91 peer review and production represents the most expensive part.
 92 Therefore, we investigated a strategy for the efficient formatting of scientific manuscripts.

93 **Current standard publishing formats**

94 Generally speaking, a scientific manuscript is composed of contents and formatting. While the content,
 95 i.e. text, figures, tables, citations etc., may remain the same between different publishing forms and jour-
 96 nal styles, the formatting can be very different. Most publishers require the formatting of submitted
 97 manuscripts in a certain format. Ignoring this **Guide for Authors**, e.g. by submitting a manuscript with
 98 a different reference style, gives a negative impression with a journal’s editorial staff. Too carelessly
 99 prepared manuscripts can even provoke a straight ‘desk-reject’ (Volmer & Stokes, 2016).

100 Currently DOC(X), LATEX and/ or PDF file formats are the most frequently used formats for journal
 101 submission platforms. But even if the content of a submitted manuscript might be accepted during the
 102 peer review ‘as is’, the format still needs to be adjusted to the particular publication style in the production
 103 stage. For the electronic distribution and archiving of scientific works, which is gaining more and more
 104 importance, additional formats (EPUB, (X)HTML, JATS) need to be generated. **Tab. 1** lists the file
 105 formats which are currently the most relevant ones for scientific publishing.

106 Although the content elements of documents, such as title, author, abstract, text, figures, tables, etc.,
 107 remain the same, the syntax of the file formats is rather different. **Tab. 2** demonstrates some simple
 108 examples of differences in different markup languages.

109 Documents with the commonly used Office Open XML (DOCX Microsoft Word files) and OpenDocu-
 110 ment (ODT LibreOffice) file formats can be opened in a standard text editor after unzipping. However,
 111 content and formatting information is distributed into various folders and files. Practically speaking, those
 112 file formats require the use of special word processing software.

113 From a writer’s perspective, the use of *What You See Is What You Get* (WYSIWYG) programs such as
 114 Microsoft Word, WPS Office or LibreOffice might be convenient, because the formatting of the document
 115 is directly visible. But the complicated syntax specifications often result in problems when using different
 116 software versions and for collaborative writing. Simple conversions between file formats can be difficult
 117 or impossible. In a worst-case scenario, ‘old’ files cannot be opened any more for lack of compatible
 118 software.

119 In some parts of the scientific community therefore LATEX, a typesetting program in plain text format,
 120 is very popular. With LATEX, documents with highest typographic quality can be produced. However,
 121 the source files are cluttered with LATEX commands and the source text can be complicated to read.
 122 Causes of compilation errors in LATEX are sometimes difficult to find. Therefore, LATEX is not very
 123 user friendly, especially for casual writers or beginners.

124 **Table 1.** Current standard formats for scientific publishing.

Type	Description	Use	Syntax	Reference
DOCX	Office Open XML	WYSIWYG editing	XML, ZIP	(Ngo, 2006)
ODT	OpenDocument	WYSIWYG editing	XML, ZIP	(Brauer et al., 2005)
PDF	portable document	print replacement	PDF	(International Organization for Standardization, 2013)
EPUB	electronic publishing	e-books	HTML5, ZIP	(Eikebrokk, Dahl & Kessel, 2014)
JATS	journal article tag suite	journal publishing	XML	(National Information Standards Organization, 2012)
LATEX	typesetting system	high-quality print	TEX	(Lamport, 1994)
HTML	hypertext markup	websites	(X)HTML	(Raggett et al., 1999; Hickson et al., 2014)
MD	Markdown	lightweight markup	plain text MD	(Ovadia, 2014; Leonard, 2016)

125 **Table 2.** Examples for formatting elements and their implementations in different markup languages.

Element	Markdown	LATEX	HTML
structure			
section	# Intro	\section{Intro}	<h1>Intro</h1>
subsection	## History	\subsection{History}	<h2>History</h2>
text style			
bold	**text**	\textbf{text}	text
italics	*text*	\textit{text}	<i>text</i>
links			
HTTP link	<https://arxiv.org>	\usepackage{url}\url{https://arxiv.org}	

126 In academic publishing, it is additionally desirable to create different output formats from the same source
 127 text:

- 128 • For the publishing of a book, with a print version in PDF and an electronic version in EPUB.
 129 • For the distribution of a seminar script, with an online version in HTML and a print version in
 130 PDF.
 131 • For submitting a journal manuscript for peer-review in DOCX, as well as a preprint version with
 132 another journal style in PDF.
 133 • For archiving and exchanging article data using the Journal Article Tag Suite (JATS) (National
 134 Information Standards Organization, 2012), a standardized format developed by the NLM.

135 Some of the tasks can be performed e.g. with LATEX, but an integrated solution remains a challenge.
 136 Several programs for the conversion between documents formats exist, such as the e-book library program
 137 calibre <http://calibre-ebook.com/>. But the results of such conversions are often not satisfactory
 138 and require substantial manual corrections.

139 Therefore, we were looking for a solution that enables the creation of scientific manuscripts in a simple
140 format, with the subsequent generation of multiple output formats. The need for hybrid publishing has
141 been recognized outside of science (Kielhorn, 2011; DPT Collective, 2015), but the requirements specific
142 to scientific publishing have not been addressed so far. Therefore, we investigated the possibility to
143 generate multiple publication formats from a simple manuscript source file.

144 CONCEPTS OF MARKDOWN AND PANDOC

145 Markdown was originally developed by John Gruber in collaboration with Aaron Swartz, with the goal
146 to simplify the writing of HTML documents <http://daringfireball.net/projects/markdown/>.
147 Instead of coding a file in HTML syntax, the content of a document is written in plain text and annotated
148 with simple tags which define the formatting. Subsequently, the Markdown (MD) files are parsed to
149 generate the final HTML document. With this concept, the source file remains easily readable and the
150 author can focus on the contents rather than formatting. Despite its original focus on the web, the MD
151 format has been proven to be well suited for academic writing (Ovadia, 2014). In particular, pandoc-
152 flavored MD (<http://pandoc.org/>) adds several extensions which facilitate the authoring of academic
153 documents and their conversion into multiple output formats. **Tab. 2** demonstrates the simplicity of MD
154 compared to other markup languages. **Fig. 3** illustrates the generation of various formatted documents
155 from a manuscript in pandoc MD. Some relevant functions for scientific texts are explained below in
156 more detail.

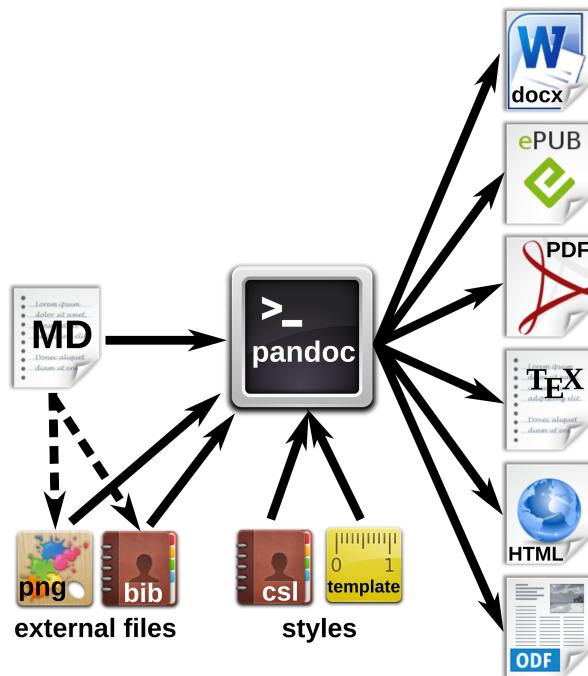


Figure 3. Workflow for the generation of multiple document formats with pandoc. The markdown (MD) file contains the manuscript text with formatting tags, and can also refer to external files such as images or reference databases. The pandoc processor converts the MD file to the desired output formats. Documents, citations etc. can be defined in style files or templates.

157 MARKDOWN EDITORS AND ONLINE EDITING

158 The usability of a text editor is important for the author, either writing alone or with several co-authors. In
159 this section we present software and strategies for different scenarios. **Fig. 4** summarizes various options
160 for local or networked editing of MD files.

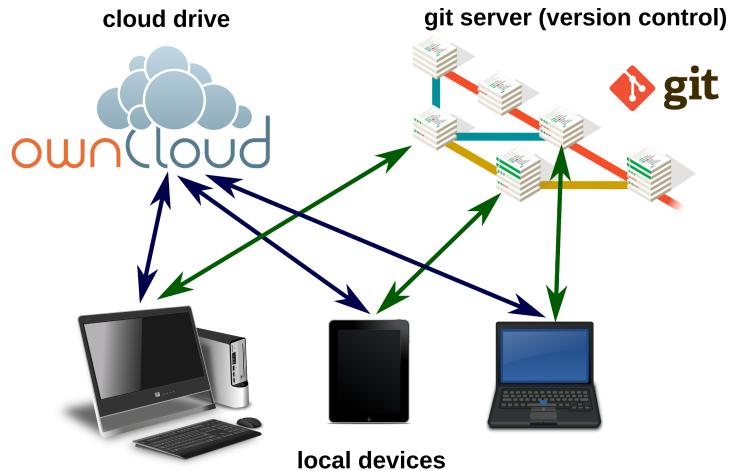


Figure 4. Markdown files can be edited on local devices or on cloud drives. A local or remote git repository enables advanced advanced version control.

161 **Markdown editors**

162 Due to MD's simple syntax, basically any text editor is suitable for editing markdown files. The formatting
 163 tags are written in plain text and are easy to remember. Therefore, the author is not distracted by looking
 164 around for layout options with the mouse. For several popular text editors, such as vim (<http://www.vim.org/>),
 165 GNU Emacs (<https://www.gnu.org/software/emacs/>), atom (<https://atom.io/>)
 166 or geany (<http://www.geany.org/>), plugins provide additional functionality for markdown editing,
 167 e.g. syntax highlighting, command helpers, live preview or structure browsing.
 168 Various dedicated markdown editors have been published as well. Many of those are cross-platform com-
 169 patible, such as Abricotine (<http://abricotine.brrd.fr/>), ghostwriter (<https://github.com/wereturtle/ghostwriter>) and CuteMarkEd (<https://choose.github.io/CuteMarkEd/>).
 170
 171 The lightweight format is also ideal for writing on mobile devices. Numerous applications are available on
 172 the App stores for Android and iOS systems. The programs Swype and Dragon (<http://www.nuance.com/>)
 173 facilitate the input of text on such devices by guessing words from gestures and speech recognition
 174 (dictation).
 175 **Fig. 5.** shows the editing of a markdown file, using the cross-platform editor Atom with several markdown
 176 plugins.

177 **Online editing and collaborative writing**

178 Storing manuscripts on network drives (*The Cloud*) has become popular for several reasons:
 179

- Protection against data loss.
- Synchronization of documents between several devices.
- Collaborative editing options.

 180 Markdown files on a Google Drive (<https://drive.google.com>) for instance can be edited online
 181 with StackEdit (<https://stackedit.io>). **Fig. 6** demonstrates the online editing of a markdown file
 182 on an ownCloud (<https://owncloud.com>) installation. OwnCloud is an Open Source software plat-
 183 form, which allows the set-up of a file server on personal webspace. The functionality of an ownCloud
 184 installation can be enhanced by installing plugins.
 185 Even mathematical formulas are rendered correctly in the HTML live preview window of the ownCloud
 186 markdown plugin (**Fig. 6**).
 187 The collaboration and authoring platform Authorea (<https://www.authorea.com>) also supports
 188 markdown as one of multiple possible input formats. This can be beneficial for collaborations in which
 189 one or more authors are not familiar with markdown syntax.

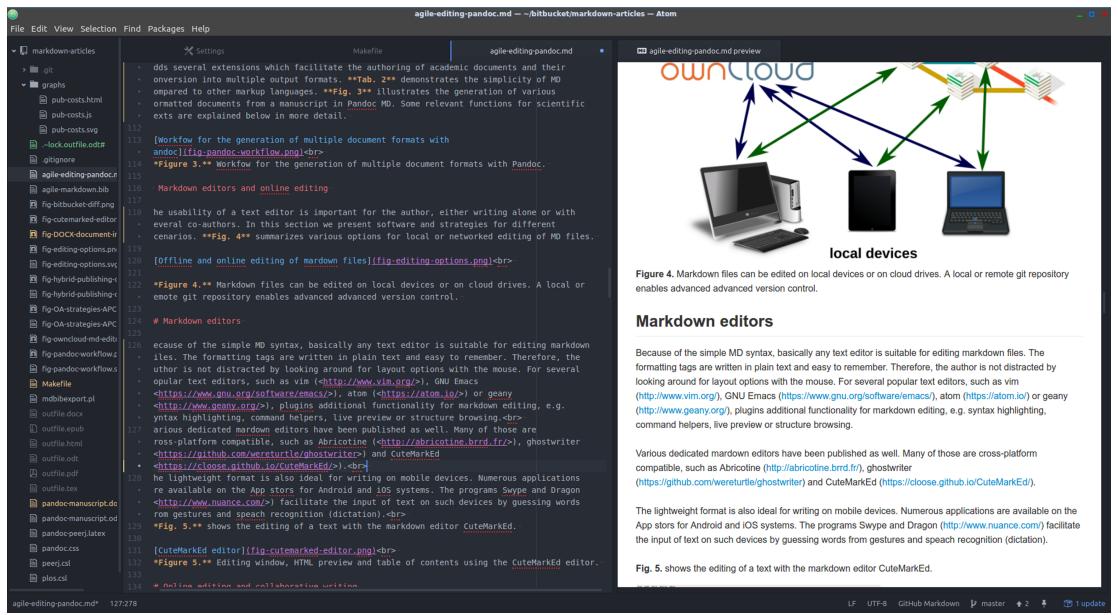


Figure 5. Document directory tree, editing window and HTML preview using the Atom editor.

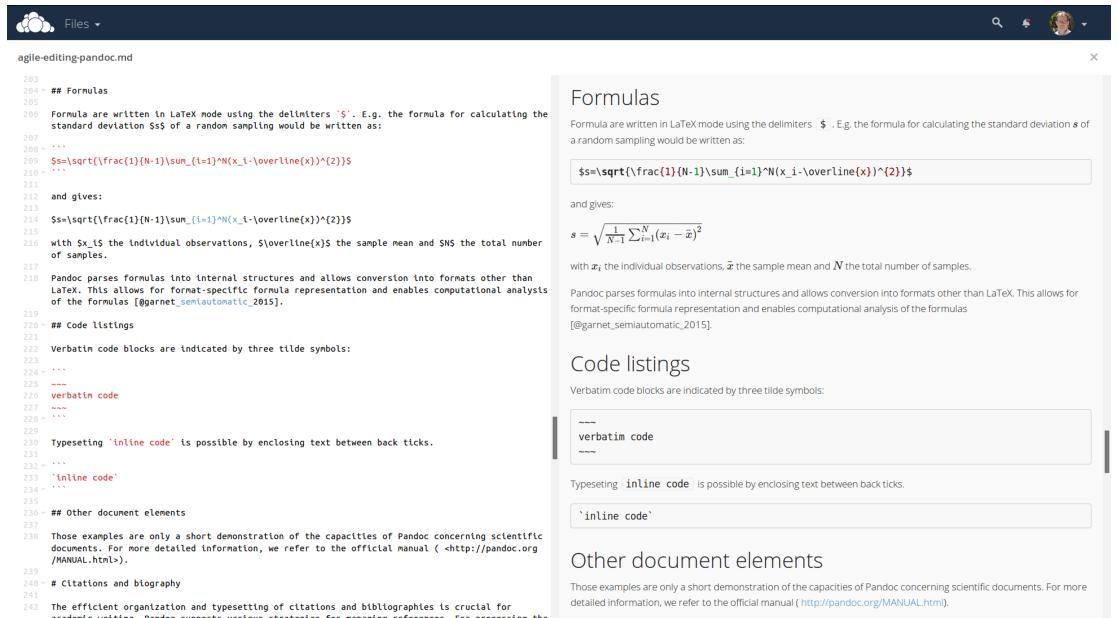


Figure 6. Direct online editing of this manuscript with live preview using the ownCloud Markdown Editor plugin by Robin Appelman.

192 **Document versioning and change control**

193 Programmers, especially when working in distributed teams, rely on version control systems to manage
 194 changes of code. Currently, Git (<https://git-scm.com/>), which is also used e.g. for the development
 195 of the Linux kernel, is one of the most employed software solutions for versioning. Git allows the parallel
 196 work of collaborators and has an efficient merging and conflict resolution system. A Git repository may
 197 be used by a single local author to keep track of changes, or by a team with a remote repository, e.g. on
 198 github (<https://github.com/>) or bitbucket (<https://bitbucket.org/>). Because of the plain text
 199 format of markdown, Git can be used for version control and distributed writing. For the writing of the
 200 present article, the co-authors (Germany and Mexico) used a remote Git repository on bitbucket. The
 201 plain text syntax of markdown facilitates the visualization of differences of document versions, as shown
 202 in **Fig. 7**.

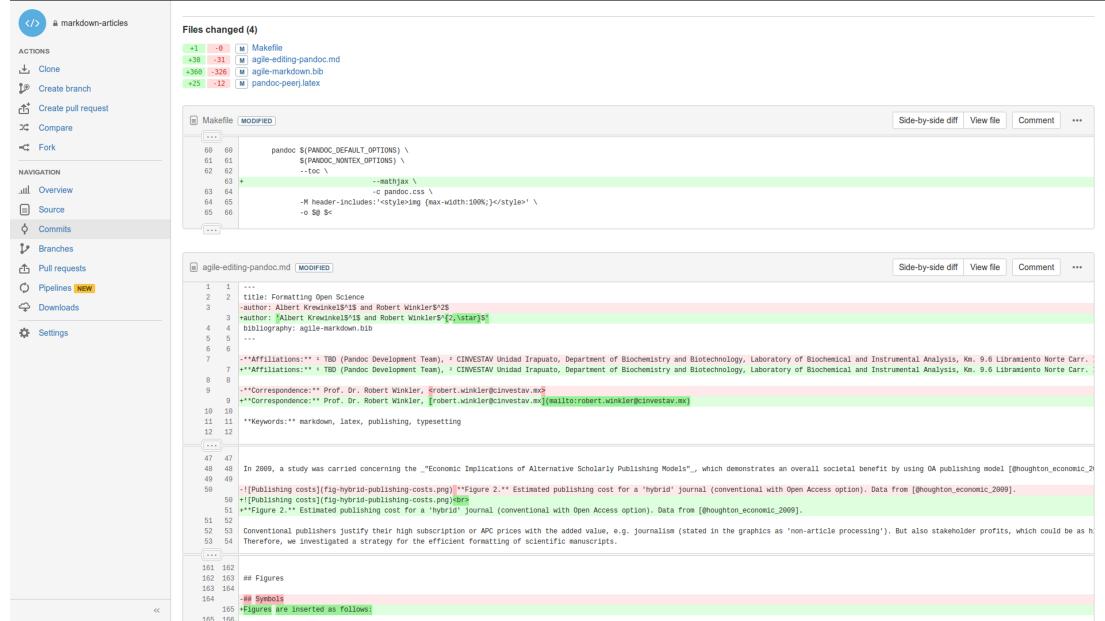


Figure 7. Version control and collaborative editing using a git repository on bitbucket.

203 **PANDOC MARKDOWN FOR SCIENTIFIC TEXTS**

204 In the following section, we demonstrate the potential for typesetting scientific manuscripts with pan-
 205 doc using examples for typical document elements, such as tables, figures, formulas, code listings and
 206 references. A brief introduction is given by Dominici (2014). The complete Pandoc User's Manual is
 207 available at <http://pandoc.org/MANUAL.html>.

208 **Tables**

209 There are several options to write tables in markdown. The most flexible alternative - which was also
 210 used for this article - are pipe tables. The contents of different cells are separated by pipe symbols (|):

211 `Left | Center | Right | Default`
 212 `-----|-----:|-----:|-----`
 213 `LLL | CCC | RRR | DDD`

214 gives

Left	Center	Right	Default
LLL	CCC	RRR	DDD

215 The headings and the alignment of the cells are given in the first two lines. The cell width is variable. The
216 pandoc parameter `--columns=NUM` can be used to define the length of lines in characters. If contents do
217 not fit, they will be wrapped.
218 Complex tables, e.g. tables featuring multiple headers or those containing cells spanning multiple rows or
219 columns, are currently not representable in markdown format. However, it is possible to embed LATEX
220 and HTML tables into the document. These format-specific tables will only be included in the output if
221 a document of the respective format is produced. This method can be extended to apply any kind of
222 format-specific typographic functionality which would otherwise be unavailable in markdown syntax.

223 **Figures and images**

224 Images are inserted as follows:

225 `! [alt text] (image location/ name)`

226 e.g.

227 `! [Publishing costs] (fig-hybrid-publishing-costs.png)`

228 The `alt text` is used e.g. in HTML output. Image dimensions can be defined in braces:

229 `! [] (fig-hybrid-publishing-costs.png)`

230 As well, an identifier for the figure can be defined with `#`, resulting e.g. in the image attributes `{#figure1`
231 `height=30%}`.

232 A paragraph containing only an image is interpreted as a figure. The `alt text` is then output as the figure's
233 caption.

234 **Symbols**

235 Scientific texts often require special characters, e.g. Greek letters, mathematical and physical symbols
236 etc.

237 The UTF-8 standard, developed and maintained by *Unicode Consortium*, enables the use of characters
238 across languages and computer platforms. The encoding is defined as RFC document 3629 of the Network
239 Working group (Yergeau, 2003) and as ISO standard ISO/IEC 10646:2014 (International Organization for
240 Standardization, 2014). Specifications of Unicode and code charts are provided on the Unicode homepage
241 (<http://www.unicode.org/>).

242 In pandoc markdown documents, Unicode characters such as `°`, `α`, `ä`, `Å` can be inserted directly and
243 passed to the different output documents. The correct processing of MD with UTF-8 encoding to LATEX/PDF
244 output requires the use of the `--latex-engine=xelatex` option and the use of an appropriate
245 font. The Times-like XITS font (<https://github.com/khaledhosny/xits-math>), suitable for high
246 quality typesetting of scientific texts, can be set in the LATEX template:

```
\usepackage{unicode-math}
\setmainfont
[ Extension = .otf,
  UprightFont = *-regular,
  BoldFont = *-bold,
  ItalicFont = *-italic,
  BoldItalicFont = *-bolditalic,
]{xits}
\setmathfont
[ Extension = .otf,
  BoldFont = *bold,
]{xits-math}
```

247 To facilitate the input of specific characters, so-called mnemonics can be enabled in some editors (e.g. in
248 atom by the `character-table` package). For example, the 2-character Mnemonics ‘:u’ gives ‘ü’ (di-
249 aeresis), or ‘D*’ the Greek Δ. The possible character mnemonics and character sets are listed in RFC
250 1345 <http://www.faqs.org/rfcs/rfc1345.html> (Simonsen, 1992).

251 **Formulas**

252 Formulas are written in LATEX mode using the delimiters \$. E.g. the formula for calculating the standard
253 deviation s of a random sampling would be written as:

254
$$s = \sqrt{\frac{1}{N-1} \sum_{i=1}^N (x_i - \bar{x})^2}$$

255 and gives:

256
$$s = \sqrt{\frac{1}{N-1} \sum_{i=1}^N (x_i - \bar{x})^2}$$

257 with x_i the individual observations, \bar{x} the sample mean and N the total number of samples.

258 Pandoc parses formulas into internal structures and allows conversion into formats other than LATEX.
259 This allows for format-specific formula representation and enables computational analysis of the formulas
260 (Corbí & Burgos, 2015).

261 **Code listings**

262 Verbatim code blocks are indicated by three tilde symbols:

263 ~~~
264 `verbatim code`
265 ~~~

266 Typesetting `inline` code is possible by enclosing text between back ticks.

267 ``inline code``

268 **Other document elements**

269 These examples are only a short demonstration of the capacities of pandoc concerning scientific docu-
270 ments. For more detailed information, we refer to the official manual (<http://pandoc.org/MANUAL.html>).

272 **CITATIONS AND BIOGRAPHY**

273 The efficient organization and typesetting of citations and bibliographies is crucial for academic writing.
274 Pandoc supports various strategies for managing references. For processing the citations and the creation
275 of the bibliography, the command line parameter `--filter pandoc-citeproc` is used, with variables
276 for the reference database and the bibliography style. The bibliography will be located automatically at
277 the header `# References` or `# Bibliography`.

278 **Reference databases**

279 Pandoc is able to process all mainstream literature database formats, such as RIS, BIB, etc. However, for
280 maintaining compatibility with LATEX/ BIBTEX, the use of BIB databases is recommended. The used
281 database either can be defined in the YAML metablock of the MD file (see below) or it can be passed as
282 parameter when calling pandoc.

283 **Inserting citations**

284 For inserting a reference, the database key is given within square brackets, and indicated by an '@'. It is
285 also possible to add information, such as page:

286 `[@suber_open_2012; @benkler_wealth_2006, 57 ff.]`

287 gives (Benkler, 2006, p. 57 ff.; Suber, 2012).

288 **Styles**

289 The Citation Style Language (CSL) <http://citationstyles.org/> is used for the citations and bibliographies.
290 This file format is supported e.g. by the reference management programs Mendeley <https://www.mendeley.com/>, Papers <http://papersapp.com/> and Zotero <https://www.zotero.org/>.
291 CSL styles for particular journals can be found from the Zotero style repository <https://www.zotero.org/styles>. The bibliography style that pandoc should use for the target document can be chosen in
292 the YAML block of the markdown document or can be passed in as a command line option. The latter
293 is more recommendable, because distinct bibliography style may be used for different documents.
294

296 **Creation of LATEX natbib citations**

297 For citations in scientific manuscripts written in LATEX, the natbib package is widely used. To create
298 a LATEX output file with natbib citations, pandoc simply has to be run with the `--natbib` option, but
299 without the `--filter pandoc-citeproc` parameter.

300 **Database of cited references**

301 To share the bibliography for a certain manuscript with co-authors or the publisher's production team, it
302 is often desirable to generate a subset of a larger database, which only contains the cited references. If
303 LATEX output was generated with the `--natbib` option, the compilation of the file with LATEX gives an
304 AUX file (in the example named `md-article.aux`), which subsequently can be extracted using BibTool
305 <https://github.com/ge-ne/bibtool>:

306 `~~~`
307 `bibtool -x md-article.aux -o bibshort.bib`
308 `~~~`

309 In this example, the article database will be called `bibshort.bib`.

310 For the direct creation of an article specific BIB database without using LATEX, we wrote a simple Perl
311 script called `mdbibexport` (<https://github.com/robert-winkler/mdbibexport>).

312 **META INFORMATION OF THE DOCUMENT**

313 Bourne (2005) argues that journals should be effectively equivalent to biological databases: both provide
314 data which can be referenced by unique identifiers like DOI or e.g. gene IDs. Applying the semantic-web
315 ideas of Berners-Lee & Hendler (2001) to this domain can make this vision a reality. Here we show how
316 metadata can be specified in markdown. We propose conventions, and demonstrate their suitability to
317 enable interlinked and semantically enriched journal articles.

318 Document information such as title, authors, abstract etc. can be defined in a metadata block written in
319 YAML syntax. YAML ("YAML Ain't Markup Language", <http://yaml.org/>) is a data serialization
320 standard in simple, human readable format. Variables defined in the YAML section are processed by
321 pandoc and integrated into the generated documents. The YAML metadata block is recognized by three
322 hyphens (---) at the beginning, and three hyphens or dots (...) at the end, e.g.:

```
---  
title: Formatting Open Science  
subtitle: agile creation of multiple document types  
date: 2017-02-10  
...  
323 The public availability of all relevant information is a central aspect of Open Science. Analogous to article  
324 contents, data should be accessible via default tools. We believe that this principle must also be applied  
325 to article metadata. Thus, we created a custom pandoc writer that emits the article's data as JSON-LD  
326 (Lanthaler & Güttl, 2012), allowing for informational and navigational queries of the journal's data with  
327 standard tools of the semantic web. The above YAML information would be output as:
```

```
{  
  "@context": {  
    "@vocab": "http://schema.org/",  
    "date": "datePublished",  
    "title": "headline",  
    "subtitle": "alternativeTitle"  
  },  
  "@type": "ScholarlyArticle",  
  "title": "Formatting Open Science",  
  "subtitle": "agile creation of multiple document types",  
  "date": "2017-02-10"  
}
```

328 This format allows processing of the information by standard data processing software and browsers.

329 **Flexible metadata authoring**

330 We developed a method to allow writers the flexible specification of authors and their respective affiliations.
331 Author names can be given as a string, via the key of a single-element object, or explicitly as a
332 name attribute of an object. Affiliations can be specified directly as properties of the author object, or
333 separately in the institute object.

334 Additional information, e.g. email addresses or identifiers like ORCID (Haak et al., 2012), can be added
335 as additional values:

```
author:  
  - John Doe:  
    institute: fs  
    email: john.doe@example.com  
    orcid: 0000-0000-0000-0000  
institute:  
  fs: Science Formatting Working Group
```

336 **JATS support**

337 The journal article tag suite (JATS) was developed by the NLM and standardized by ANSI/NISO as
338 an archiving and exchange format of journal articles and the associated metadata (National Information
339 Standards Organization, 2012), including data of the type shown above. The pandoc-jats writer by
340 Martin Fenner is a plugin usable with pandoc to produce JATS-formatted output. The writer was adapted
341 to be compatible with our metadata authoring method, allowing for simple generation of files which
342 contain the relevant metadata.

343 **Citation types**

344 Writers can add information about the reason a citation is given. This might help reviewers and readers,
345 and can simplify the search for relevant literature. We developed an extended citation syntax that inte-

346 grates seamlessly into markdown and can be used to add complementary information to citations. Our
347 method is based on CiTO, the Citation Typing Ontology (Shotton, 2010), which specifies a vocabulary
348 for the motivation when citing a resource. The type of a citations can be added to a markdown citation using
349 `@CITO_PROPERTY:KEY`, where `CITO_PROPERTY` is a supported CiTO property, and `KEY` is the usual
350 citation key. Our tool extracts that information and includes it in the generated linked data output. A
351 general CiTO property (`cites`) is used, if no CiTO property is found in a citation key.

352 The work at hand will always be the subject of the generated semantic *subject-predicate-object* triples.
353 Some CiTO predicates cannot be used in a sensical way under this condition. Focusing on author convenience,
354 we use this fact to allow shortening of properties when sensible. E.g. if authors of a biological
355 paper include a reference to the paper describing a method which was used in their work, this relation
356 can be described by the `uses_method_in` property of the CiTO ontology. The inverse property, `pro-`
357 `vides_method_for`, would always be nonsensical in this context as implied by causality. It is therefore not
358 supported by our tool. This allows us to introduce an abbreviation (`method`) for the latter property, as any
359 ambiguity has been eliminated. Users of western blotting might hence write `@method_in:towbin_1979`
360 or even just `@method:towbin_1979`, where `towbin_1979` is the citation identifier of the describing paper
361 by Towbin, Staehelin & Gordon (1979).

362 **EXAMPLE: MANUSCRIPT WITH OUTPUT OF DOCX/ ODT FORMAT 363 AND LATEX/ PDF FOR SUBMISSION TO DIFFERENT JOURNALS.**

364 Scientific manuscripts have to be submitted in a format defined by the journal or publisher. At the moment,
365 DOCX is the most common file format for manuscript submission. Some publishers also accept or require
366 LATEX or ODT formats. Additional to the general style of the manuscript - organization of sections,
367 fonts, etc. – the citation style of the journal must also be followed. Often, the same manuscript has to be
368 prepared for different journals, e.g. if the manuscript was rejected by a journal and has to be formatted
369 for another one, or if a preprint of the paper is submitted to an archive that requires a distinct document
370 format than the targeted peer-reviewed journal. In this example, we want to create a manuscript for a
371 *PLoS* journal in DOCX and ODT format for WYSIWYG word processors. Further, a version in LATEX/
372 PDF should be produced for PeerJ submission and archiving at the PeerJ preprint server.

373 The examples for DOCX/ ODT are kept relatively simple, to show the proof-of-principle and to provide a
374 plain document for the development of own templates. Nevertheless, the generated documents should be
375 suitable for submission after little manual editing. For specific journals it may be necessary to create more
376 sophisticated templates or to copy/ paste the generic DOCX/ ODT output into the publisher's template.

377 **Development of a DOCX/ ODT template**

378 A first DOCX document with bibliography in *PLoS* format is created with pandoc DOCX output:

```
pandoc -S -s --csl=plos.csl --filter pandoc-citeproc  
      -o pandoc-manuscript.docx agile-editing-pandoc.md
```

379 The parameters `-S` `-s` generate a typographically correct (dashes, non-breaking spaces etc.) stand-alone
380 document. A bibliography with the *PLoS* style is created by the `citeproc` filter setting `--csl=plos.csl`
381 `--filter` `pandoc-citeproc`.

382 The document settings and styles of the resulting file `pandoc-manuscript.docx` can be optimized and
383 be used again as document template (`--reference-docx=pandoc-manuscript.docx`).

```
pandoc -S -s --reference-docx=pandoc-manuscript.docx --csl=plos.csl  
      --filter pandoc-citeproc -o outfile.docx agile-editing-pandoc.md
```

384 It is also possible to directly re-use a previous output file as template (i.e. template and output file have
385 the same file name):

```
pandoc -S -s --columns=10 --reference-docx=pandoc-manuscript.docx  
      --csl=plos.csl --filter=pandoc-citeproc  
      -o pandoc-manuscript.docx agile-editing-pandoc.md
```

386 In this way, the template can be incrementally adjusted to the desired document formatting. The final
387 document may be employed later as pandoc template for other manuscripts with the same specifications.
388 In this case, running pandoc the first time with the template, the contents of the new manuscript would
389 be filled into the provided DOCX template. A page with DOCX manuscript formatting of this article is
390 shown in **Fig. 8**.

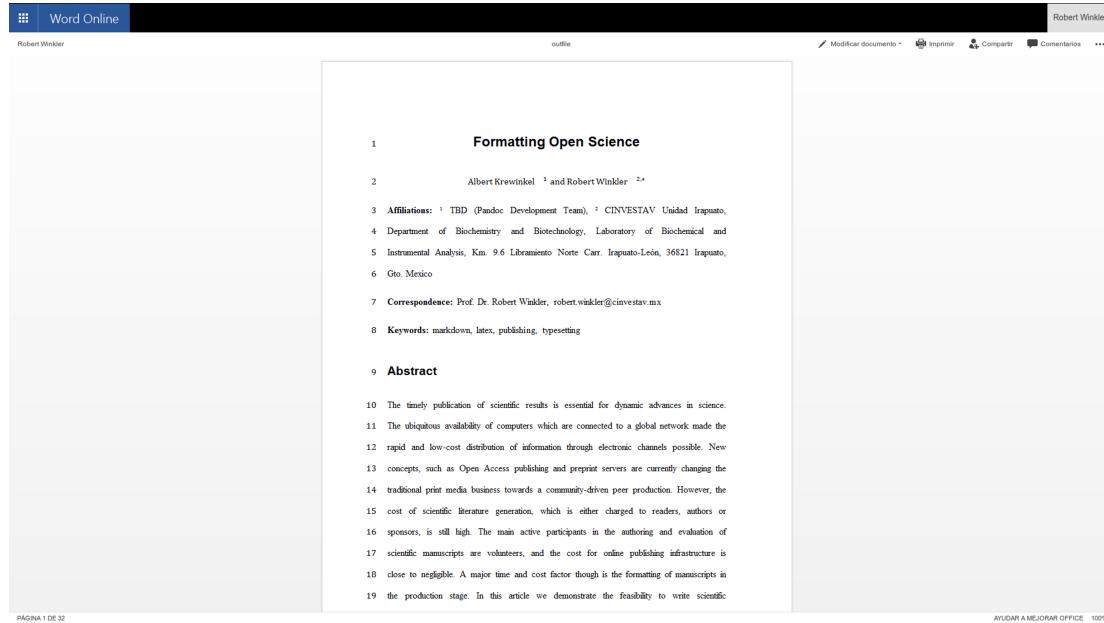


Figure 8. Opening a pandoc-generated DOCX in Microsoft Office 365.

391 The same procedure can be applied with an ODT formatted document.

392 **Development of a TEX/PDF template**

393 The default pandoc LATEX template can be written into a separate file by:

```
394 pandoc -D latex > template-peerj.latex
```

395 This template can be adjusted, e.g. by defining Unicode encoding (see above), by including particular
396 packages or setting document options (line numbering, font size). The template can then be used with
397 the pandoc parameter **--template=pandoc-peerj.latex**.

398 The templates used for this document are included as Supplemental Material (see section *Software and*
399 *code availability* below).

400 **Styles for HTML and EPUB**

401 The style for HTML and EPUB formats can be defined in .css stylesheets. The Supplemental Material
402 contains a simple example .css file for modifying the HTML output, which can be used with the pandoc
403 parameter **-c pandoc.css**.

404 **AUTOMATING DOCUMENT PRODUCTION**

405 The commands necessary to produce the document in a specific formats or styles can be defined in a
406 simple **Makefile**. An example **Makefile** is included in the source code of this preprint. The desired
407 output file format can be chosen when calling **make**. E.g. **make outfile.pdf** produces this preprint in
408 PDF format. Calling **make** without any option creates all listed document types. A **Makefile** producing
409 DOCX, ODT, JATS, PDF, LATEX, HTML and EPUB files of this document is provided as Supplemental
410 Material.

410 **Cross-platform compatibility**

411 The make process was tested on Windows 10 and Linux 64 bit. All documents – DOCX, ODT, JATS,
412 LATEX, PDF, EPUB and HTML – were generated successfully, which demonstrates the cross-platform
413 compatibility of the workflow.

414 **PERSPECTIVE**

415 Following the trend to peer production, the formatting of scientific content must become more efficient.
416 Markdown/ pandoc has the potential to play a key role in the transition from proprietary to community-
417 driven academic production. Important research tools, such as the statistical computing and graph-
418 ics language R (R Core Team, 2014) and the Jupyter notebook project (Kluyver et al., 2016) have al-
419 ready adopted the MD syntax (e.g. <http://rmarkdown.rstudio.com/>). The software for writing
420 manuscripts in MD is mature enough to be used by academic writers. Therefore, publishers also should
421 consider implementing the MD format into their editorial platforms.

422 **CONCLUSIONS**

423 Authoring scientific manuscripts in markdown (MD) format is straight-forward, and manual formatting is
424 reduced to a minimum. The simple syntax of MD facilitates document editing and collaborative writing.
425 The rapid conversion of MD to multiple formats such as DOCX, LATEX, PDF, EPUB and HTML can
426 be done easily using pandoc, and templates enable the automated generation of documents according to
427 specific journal styles.

428 The additional features we implemented facilitate the correct indexing of meta information of journal
429 articles according to the ‘semantic web’ philosophy.

430 Altogether, the MD format supports the agile writing and fast production of scientific literature. The
431 associated time and cost reduction especially favours community-driven publication strategies.

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436 **SOFTWARE AND CODE AVAILABILITY**

437 The relevant software for creating this manuscript used is cited according to (Smith, Katz & Niemeyer,
438 2016) and listed in **Tab. 3**. Since unique identifiers are missing for most software projects, we only refer
439 to the project homepages or software repositories:

440 **Table 3.** Relevant software used for this article.

Software	Use	Authors	Version		Release	Homepage/ repository
			1.16.0.2	16/01/13	http://www.pandoc.org	
pandoc	universal markup converter	John MacFarlane	1.16.0.2	16/01/13	http://www.pandoc.org	
pandoc-citeproc	library for CSL citations with pandoc	John MacFarlane, Andrea Rossato	0.9.1	16/03/19	https://github.com/jgm/pandoc-citeproc	
pandoc-jats	creation of JATS files with pandoc	Martin Fenner	0.9	15/04/26	https://github.com/mfenner/pandoc-jats	
ownCloud	personal cloud software	ownCloud GmbH, Community	9.1.1	16/09/20	https://owncloud.org/	
Editor	Markdown plugin for ownCloud	Robin Appelman	0.1	16/03/08	https://github.com/icewind1991/files_markdown	
BibTool	Bibtex database tool	Gerd Neugebauer	2.63	16/01/16	https://github.com/ge-ne/bibtool	

441 The software created as part of this article, *pandoc-scholar*, is suitable for general use and has been pub-
442 lished at <https://github.com/pandoc-scholar/pandoc-scholar>, DOI: 10.5281/zenodo.376761.
443 The source code of this manuscript, as well as the templates and pandoc Makefile, have been deposited
444 to <https://github.com/robert-winkler/scientific-articles-markdown/>.

445 Drawings for document types, devices and applications have been adopted from Calibre <http://calibre-ebook.com/>, openclipart <https://openclipart.org/> and the GNOME Theme Faenza
446 <https://code.google.com/archive/p/faenza-icon-theme/>.

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