Example of Converted Jupyter Notebook

Formatting Markdown Cells

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Converted using IPyPublish
('latex_ipypublish_all.exec').

Institution1
Institution2

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1 Writing Markdown

In IPyPublish, all Markdown content is converted *via* Pandoc. Pandoc alllows for filters to be applied to the intermediary representation of the content, which IPyPublish supplies through a group of panflute filters, wrapped in a single 'master' filter; `ipubpandoc`. This filter extends the common markdown syntax to:

- Correctly translate pieces of documentation written in other formats (such as using LaTeX commands like `\cite` or RST roles like `:cite:`)
- Handle labelling and referencing of figures, tables and equations, and add additional formatting options.

`ipubpandoc` is detached from the rest of the notebook conversion process, and so can be used as a standalone process on any markdown content:

```
$ pandoc -f markdown -t html --filter ipubpandoc path/to/file.md
```

1.1 Converting Notebooks to RMarkdown

RMarkdown is a plain text representation of the workbook. Thanks to jupytext, we can easily convert an existing notebooks to RMarkdown (and back):

```
$ jupytext --to rmarkdown notebook.ipynb
$ jupytext --to notebook notebook.Rmd            # overwrite notebook.ipynb (remove outputs)
$ jupytext --to notebook --update notebook.Rmd   # update notebook.ipynb (preserve outputs)
```

Alternatively, simply create a notebook.Rmd, and add this to the top of the file:

```
---
jupyter:
  ipub:
    pandoc:
      convert_raw: true
      hide_raw: false
      at_notation: true
      use_numref: true
  jupytext:
    metadata_filter:
      notebook: ipub
    text_representation:
      extension: .Rmd
      format_name: rmarkdown
      format_version: '1.0'
      jupytext_version: 0.8.6
  kernelspec:
    display_name: Python 3
    language: python
    name: python3
---
```

important
To preserve ipypublish notebook metadata, you must add: `{"jupytext": {"metadata_filter":`

`{"notebook": "ipub"}}}` to your notebooks metadata before conversion.

note

If a file with a .Rmd extension is supplied to `nbpublish`, it will automatically call `jupytext` and convert it. So it is possible to only ever write in the RMarkdown format!

seealso

Using YAML metadata blocks in Pandoc.

??

1.2 Working with RMarkdown files

The recommended way to edit RMarkdown files is in Visual Studio Code, with the Markdown Preview Enhanced extension. Add this to your VS Code Settings:

```
{
    "files.associations": {
        "*.Rmd": "markdown"
    },
    "markdown-preview-enhanced.usePandocParser": true,
    "markdown-preview-enhanced.pandocArguments": "--filter=ipubpandoc",
    "markdown-preview-enhanced.enableScriptExecution": true
}
```

If you are using a Conda environment, you may also need to use:

```
{
    "markdown-preview-enhanced.pandocPath": "/anaconda/envs/myenv/bin/pandoc",
    "markdown-preview-enhanced.pandocArguments": "--filter=/anaconda/myenv/lsr/bin/ipubpandoc"
}
```

You will now be able to open a dynamic preview of your notebook, with executable code cells:

```
print(1)
```

```
1
```

seealso

VS Code Extensions: Markdown Extended and markdownlint

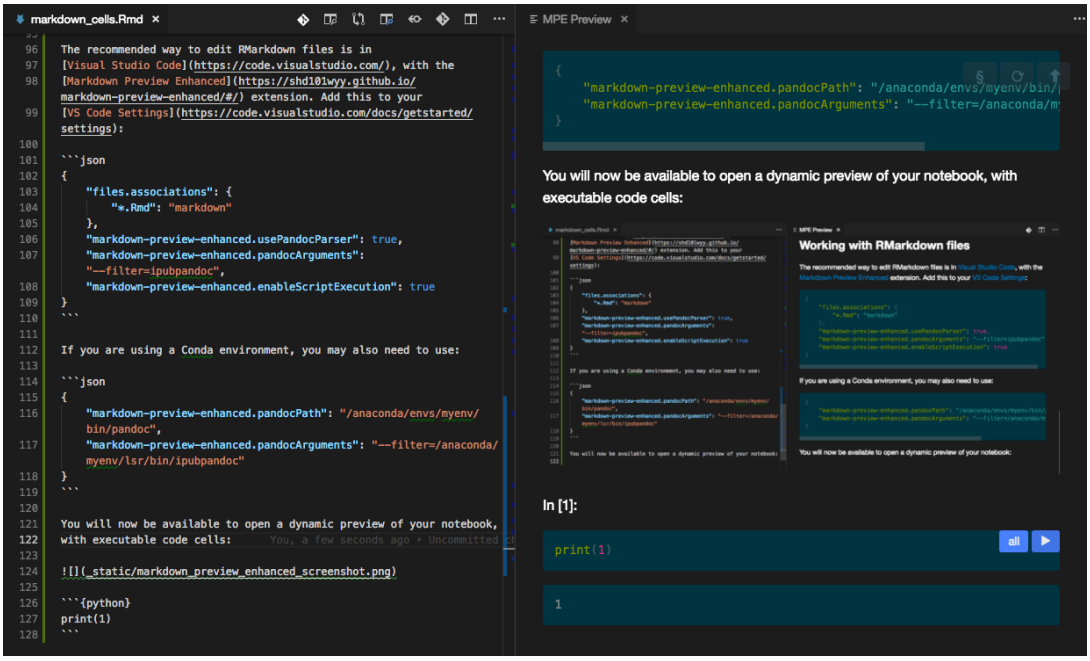

Figure 1.1: MPE Screenshot

1.3 Inter-Format Translation

`ipubpandoc` attempts to detect any segments of documentation written in LaTeX or Sphinx reStructuredText (and HTML citations), and convert them into a relevant panflute element.

Because of this we can write something like this:

```
- citations in @ notation [@zelenyak_molecular_2016; @kirkeminde_thermodynamic_2012]
- citations in rst notation :cite:`zelenyak_molecular_2016,kirkeminde_thermodynamic_2012`
- citations in latex notation \cite{zelenyak_molecular_2016,kirkeminde_thermodynamic_2012}
- citation in html notation \cite{kirkeminde_thermodynamic_2012}

$$a = b + c$$ {#eqnlabel}

- a reference in @ notation =@eqnlabel {.capital}
- a reference in rst notation :eq:`eqnlabel`
- a reference in latex notation \eqref{eqnlabel}

.. note::

    a reference in latex notation within an RST directive \eqref{eqnlabel}
```

and it will be correctly resolved in the output document:

- citations in @ notation[1,2]
- citations in rst notation[1,2]
- citations in latex notation[1,2]
- citation in html notation[2]

$$a = b + c \tag{1.1}$$

- a reference in @ notation (1.1)

- a reference in rst notation (1.1)
- a reference in latex notation (1.1)

note
a reference in latex notation within an RST directive (1.1)

Inter-format translation is turned on by default, but if you wish to turn it off, or hide it, simply add to the document metadata:

```
jupyter:
  ipub:
    pandoc:
      convert_raw: true
      hide_raw: false
```

1.4 Labelling, Formatting and Referencing Figures, Tables and Equations

`ipubpandoc` allows for figures, tables, equations and references to be supplied with an 'attribute container'. This is a braced section to the side of the figures, equations, reference or table caption, that parses on additional information to the formatter, e.g. `{#id .class-name attribute1=10}`.

Attribute containers are turned on by default, but if you wish to turn them off, simply add to the document metadata:

```
jupyter:
  ipub:
    pandoc:
      at_notation: false
```

tip
Zero or more Space is generally allowed between the element and the attribute container.

1.4.1 Figures

Figures can have an identifier and a width or height. Additionally, `placement` will be used by LaTeX output.

```
![Image caption](markdown_cells_files/example.jpg){#fig:example width=50% placement='H'}

@fig:example
```

Figure 1.2: Image caption

1.4.2 Tables

Tables can have an identifier and relative widths (per column). Additionally, `align` will be used by LaTeX and HTML to set the alignment of the columns (l=left, r=right, c=center)

Table 1.1: Table caption

	Column 1	Column 2
	1	2

1.4.3 Equations

Equations can have an identifier and an `env` denoting the amsmath environment.

```
$$2x &=  8 \\ 3x + 9y &= -12$$ {#eqn:example2 env=align}
```

$$2x = 8 \tag{1.2}$$
$$3x + 9y = -12 \tag{1.3}$$

note
Labelled math must be 'display math', rather than inline, i.e. wrapped in double dollars.

1.4.4 References

Pandoc references are start with @ and multiple references can be wrapped in square brackets:

```
Citation [@zelenyak_molecular_2016; @kirkeminde_thermodynamic_2012]
```

Citation[1,2]

References can have attributes; `latex` (defining the LaTeX tag to use), `rst` (defining the RST role to use) and class `.capital` (defining if HTML naming if capitalized)

```
@fig:example {.capital latex=cref rst=numref}, [@eqnlabel;@eqn:example2] {latex=eqref rst=eq}
```

fig. 1.2, (1.1) and (1.3)

A number of prefixes are available, as shorthand's to define attributes:

Table 1.2: Prefixes for reference attributes

prefix	attribute
""	{latex=cite rst=cite}
"+"	{latex=cref rst=numref}
"!"	{latex=ref rst=ref}
"="	{latex=eqref rst=eq}
"?"	{.capital latex=Cref rst=numref}

```
?@fig:example, =[@eqnlabel;@eqn:example2]
```

Figure 1.2, (1.1) and (1.3)

tip
Pandoc interprets `(@label)` as a numbered example, so instead use `(@label{})`

1.5 A Note on Implementation

To assign attributes to items, we use a preparation filter, to extract prefixes and attributes, and wrap the items in a Span containing them. For example:

```
$$a=1$$ {#a env=align}
```

will be transformed to:

```
<p>
<span id="a" class="labelled-Math" data-env="align">
<br />
<span class="math display">
<em>a</em> = 1
</span>
<br />
</span>
</p>
```

and

```
"+@label{ .class a=1} xyz *@label2* @label3{ .b}"
```

will be transformed to:

```
<p>
<span class="attribute-Cite class"
data-latex="cref" data-rst="numref" data-a="1">
<span class="citation" data-cites="label">
@label
```

```
</span></span>
xyz
<em><span class="citation" data-cites="label2">
@label2
</span></em>
<span class="attribute-Cite b">
<span class="citation" data-cites="label3">
@label3
</span></span>
</p>
```

Formatter filters, then look for these parent spans, to provide identifiers, classes and attributes.

2 References

[1] T. Yu Zelenyak, Kh T. Kholmurodov, A. R. Tameev, A. V. Vannikov, and P. P. Gladyshev. Molecular dynamics study of perovskite structures with modified interatomic interaction potentials. *High Energy Chemistry*, 50(5):400–405, 2016. ISSN 0018-1439, 1608-3148. doi:10.1134/S0018143916050209.

[2] Alec Kirkeminde and Shenqiang Ren. Thermodynamic control of iron pyrite nanocrystal synthesis with high photoactivity and stability. *Journal of Materials Chemistry A*, 1(1):49–54, 2012. ISSN 2050-7496. doi:10.1039/C2TA00498D.