Publishing Notebooks Using JATS and MECA

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Scope

JATS

- Referencing notebooks used as source for entire article
- Referencing notebooks used to produce figures, tables, etc.

MECA

- Bundling notebooks into MECA archives
- Referencing notebook source code in MECA

Notebooks in JATS XML

Notebooks in Article Metadata

Include notebooks associated with the article as supplementary material in <article-metadata>

```
1 <article-meta>
2 <article-id pub-id-type="pmid">10092260</article-id>
3 ...
4 <supplementary-material id="nb-sup-1"
5 xlink:href="notebooks/source.ipynb"
6 specific-use="document"
7 mimetype="application/x-ipynb+json"/>
8 </article-meta>
```

- Use <supplementary-material> to reference
- Include all notebooks associated with article (the document source notebook as well as source notebooks)
- Use specific-use attribute to differentiate document, supporting, or output notebooks (document, source, supporting)

<alternatives/>

Use the <alternatives> element to provide notebook references for figures, tables, etc.



- Contains processing alternatives for a given element
- Referenceable via <xref>
- Include notebook as <media> or <supplementary-material>

<media>

Approach 1: Use media to provide notebooks as alternatives for body, fig, and table-wrap elements.

1	<fig id="f3" position="float"></fig>
2	<alternatives></alternatives>
3	<pre><graphic></graphic></pre>
4	<media <="" id="nb-cell-id" th=""></media>
5	<pre>mimetype="application/x-ipynb+json"</pre>
6	<pre>specific-use="source-notebook"</pre>
7	<pre>xlink:href="notebooks/source.ipynb#cell-id"/></pre>
8	
9	
10	<table-wrap></table-wrap>
11	<alternatives></alternatives>
12	
13	<media <="" id="nb-cell-id-tbl" th=""></media>
14	<pre>mimetype="application/x-ipynb+json"</pre>
15	<pre>specific-use="source-notebook"</pre>
16	<pre>xlink:href="notebooks/source.ipynb#cell-id-tb</pre>
17	
18	

- Pointer to non-XML object
- Object is considered integral to article
- href includes cell identifier

<supplementary-material>

Approach 2: Use supplementary-material to provide notebooks as alternatives for body, fig, and table-wrap elements.

1	<fig id="f3" position="float"></fig>	
2	<alternatives></alternatives>	
3	<pre><graphic></graphic></pre>	
4	<supplementary-material <="" id="nb-sup-1" th=""></supplementary-material>	
5	<pre>xlink:href="notebooks/source.ipynb#cell-id"</pre>	
6	<pre>mimetype="application/x-ipynb+json"></pre>	
7	<caption></caption>	
8	source notebook for this figure	
9		
10		
11		
12		
13	<table-wrap></table-wrap>	
	-	
14	<alternatives></alternatives>	
14 15	<alternatives> </alternatives>	
14 15 16	<alternatives> <supplementary-material <="" id="nb-sup-2" th=""></supplementary-material></alternatives>	
14 15 16 17	<pre><alternatives> <supplementary-material <="" id="nb-sup-2" pre="" xlink:href="notebooks/source.ipynb#cell-id2"></supplementary-material></alternatives></pre>	
14 15 16 17 18	<pre><alternatives> <supplementary_material id="nb-sup-2" mimetype="application/x-ipynb+json" xlink:href="notebooks/source.ipynb#cell-id2"></supplementary_material></alternatives></pre>	
14 15 16 17 18 19	<pre><alternatives> <supplementary-material id="nb-sup-2" mimetype="application/x-ipynb+json" xlink:href="notebooks/source.ipynb#cell-id2"> <caption></caption></supplementary-material></alternatives></pre>	
14 15 16 17 18 19 20	<pre><alternatives> <alternatives> <supplementary-material id="nb-sup-2" mimetype="application/x-ipynb+json" xlink:href="notebooks/source.ipynb#cell-id2"> <caption> source notebook for this table</caption></supplementary-material></alternatives></alternatives></pre>	
14 15 16 17 18 19 20 21	<pre><alternatives> <alternatives> <supplementary-material id="nb-sup-2" mimetype="application/x-ipynb+json" xlink:href="notebooks/source.ipynb#cell-id2"> <caption x-ipynb+json"=""> <caption> source notebook for this table </caption></caption></supplementary-material></alternatives></alternatives></pre>	
14 15 16 17 18 19 20 21 22	<pre><alternatives> <tuble> <supplementary-material id="nb-sup-2" mimetype="application/x-ipynb+json" xlink:href="notebooks/source.ipynb#cell-id2"> <caption x-ipynb+json"=""> <caption x-ipynb+json"=""> <caption x-ipynb+json"=""> <caption> </caption> </caption> </caption></caption></supplementary-material></tuble></alternatives></pre>	
14 15 16 17 18 19 20 21 22 23	<pre><alternatives> <tuble> <supplementary-material id="nb-sup-2" mimetype="application/x-ipynb+json" xlink:href="notebooks/source.ipynb#cell-id2"></supplementary-material></tuble></alternatives></pre>	

- External resource that supports the article but which is not integral
- Used to add detail, background, or context to an article
- Can appear in
 <article-meta> or in
 the flow of content

Notebook href

When referencing a notebook, hrefs may optionally include a fragment which addresses a specific cell within a notebook

For example:

```
1 <supplementary-material
2 ...
3 xlink:href="notebooks/plot-src.ipynb#cell-id-1"
4 />
```

Fragments are resolved against notebooks using the following, in order:

- 1. **Cell Id**: the cell having the identifier
- 2. Cell Tags: the first cell tagged with the identifier

MECA and Notebooks

V1: Basic Notebook Support

- Include notebooks within MECA bundles
- Notebooks properly referenced from manifest.xml
- Notebooks referenced from within article.xml file via JATS XML
- By convention, place referenced notebooks within a notebooks subfolder

V2: Notebook Execution Support

- Add a notebooks.xml (notebook manifest) file to MECA bundle
- Optionally contains url to live interactive version
- Optionally includes a <source/> which provides ability to recreate execution environment

```
1 <notebook url='notebooks/document.ipynb'
2 deploy='(uri-to-live-interactive-version)'>
3 <source path='(local-REES-path)|(remote-repo-path)' type='REES'/>
4 <notebook>
```

- source points to a local or remote path which can be used to recreate the execution environment for the notebook
 - REES Compliant local or remote path
 - Path to local container or remote container registry
- By convention, place local sources in a source folder

Open Question: Review

- Reviewers likely need a Word or PDF copy of the article for review
- Bundling rendered copies within MECA is straightforward, however links to notebooks are an open question

Appendix - Complete Example

Sample JATS

Simple article created using a note and include a figure generated using a notebook.

```
1 <?xml version="1.0" encoding="utf-8"?>
 2 <! DOCTYPE article PUBLIC "-//NLM//DTD JATS (Z39.96) Journal Archiving and Interchange DTD
 3 v1.2 20190208//EN" "https://jats.nlm.nih.gov/archiving/1.2/JATS-archivearticle1.dtd">
   <article-meta>
 4
 5
     <supplementary-material id="nb-sup-1"
 6
       xlink:href="notebooks/document.ipynb"
       specific-use="document"
 7
       mimetype="application/x-ipynb+json"/>
 8
     <supplementary-material id="nb-sup-1"
 9
       xlink:href="notebooks/source.ipynb"
10
       specific-use="source"
11
       mimetype="application/x-ipynb+json"/>
12
13
   </article-meta>
14 <article>
15
     <body>
       <fig id="f3" position="float">
16
17
       <alternatives>
           <graphic ...>...</graphic>
18
           <supplementary-material id="nb-sup-1"</pre>
19
               xlink:href="notebooks/source.ipynb#cell-id"
20
               mimetype="application/x-ipynb+json">
21
           </supplementary-material>
22
       </alternatives>
23
24
       </fig>
25
     </body>
26 </article>
```

Sample MECA Zip Contents

Notebook and environment data included to allow execution of notebooks

File Name	File Type
123e4567-e89b-12d3-a456-426655440000-	Archive file
MECA.zip	
manifest.xml	Manifest metadata file
demoarticle.xml	Article metadata file
<pre>demoarticle_files/fig-jats/plot.jpg</pre>	File uploaded by author
<pre>demoarticle_files/fig-jats/plto2.jpg</pre>	File uploaded by author
demoarticle.pdf	System file
notebooks.xml	Notebook metadata file
notebooks/source.ipynb	Notebook file (source of plot)
notebooks/article.ipynb	Notebook file (document)
source/requirements.txt	REES compliant folder

Sample notebooks.xml

Notebooks manifest

```
1 <?xml version="1.0" encoding="UTF-8"?>
2 <!DOCTYPE manifest PUBLIC "-//MECA//DTD Manifest v2.0//en" "MECA manifest.dtd">
 3
 4
   <notebooks
     xmlns="https://www.manuscriptexchange.org/schema/notebook"
 5
     notebook-version="1.0">
 6
 7
     <notebook url='notebooks/document.ipynb'
 8
               deploy='https://colab.research.google.com/drive/doc'>
 9
       <source path='source/' type='REES'/>
10
     </notebook>
11
12
     <notebook url='notebooks/source.ipynb'
13
             deploy='https://colab.research.google.com/drive/source'>
14
       <source path='source/' type='REES'/>
15
     </notebook>
16
17
18 </notebooks>
```