Using Jupyter Notebooks, MyST Markdown, & Sphinx to Publish Professional Quality HTML & LaTeX Documents

N. L. Dentinger-Anderson, C. L. Dentinger-Valentine

Jan 08, 2024

CONTENTS:

```
title: Automating Setup
description: This Notebook will illustrate how we can automate the build␣
↪of this entire Jupyter setup in a custom conda environment.
date: 2024-01-05
```

```
%%html
<style>
    body {
        --vscode-font-family: "lmroman17-regular"
    }
</style>
```

```
<IPython.core.display.HTML object>
```

CHAPTER

ONE

HOW TO AUTOMATE PYTHON ENVIRONMENT

Objective

Create a custom Conda environment and integrate into Jupyter Notebooks with a single command.

1.1 Outline of Project

I want to automate the steps that it took to configure the Lua Programming/Jupyter Notebook `conda` environment as there were a few annoying bits to the installation. I would like to prevent such hiccups in the future and also learn how to create build scripts for future environments instead of always installing programs and packages to my global/base environment.

1.1.1 Prerequisites

- User has `conda` installed on their system.
- User will want to specify the Python version every time they create a new environment.

1.1.2 Actions of Program

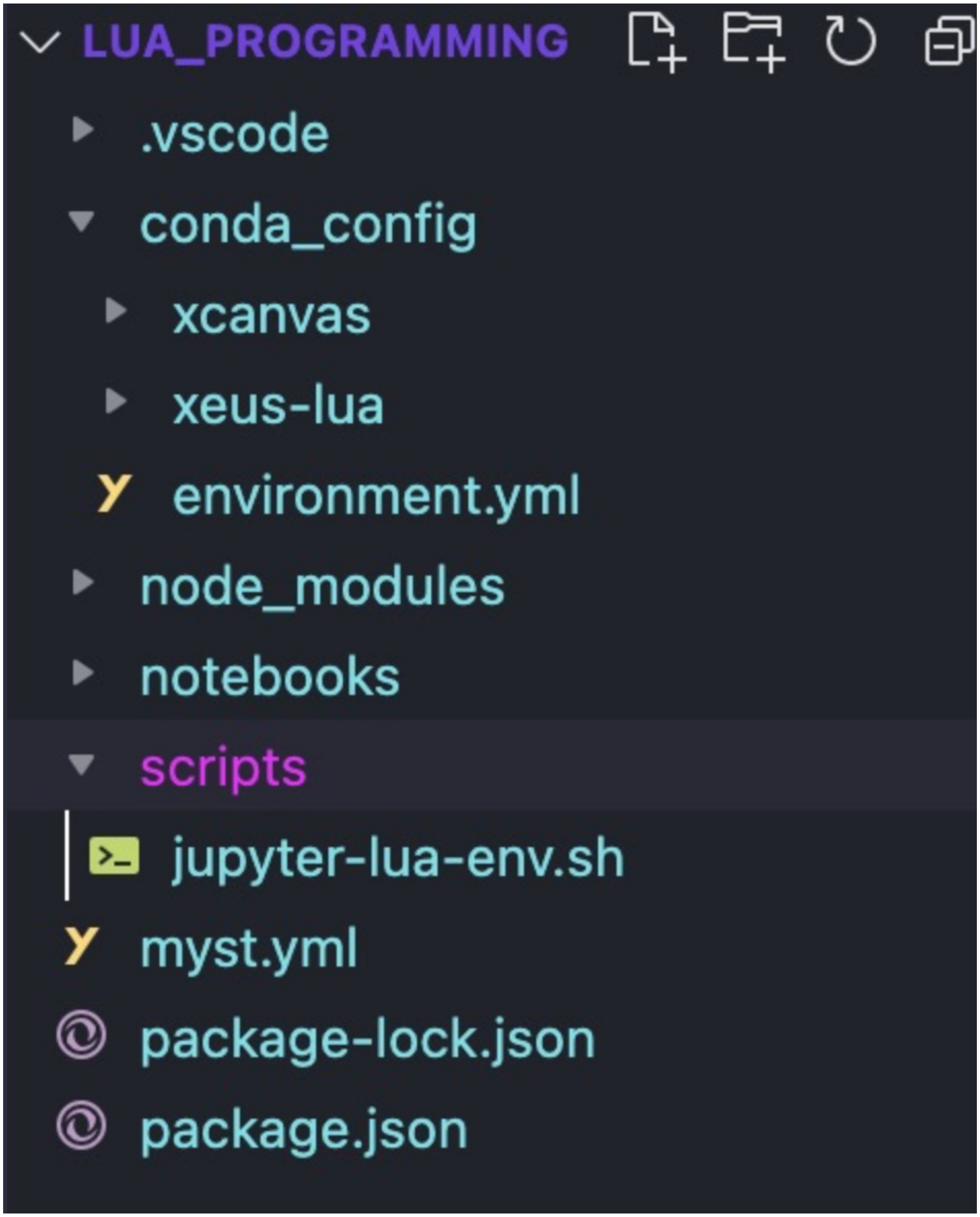
- Create environment of specified name and Python version.
- Install `ipykernel` to the Python environment.
- Link environment to Jupyter kernel.

Once all of these actions are complete, we can then activate the environment and install whatever packages we need and immediately use them in Jupyter.

1.2 Developing the Script

First, in the root directory, create a new folder called `scripts`. This will allow us to put any other scripts we make in this folder as well. Let's create two scripts `01-create-env.sh` and `02-build-env.sh`.

Assuming this root directory is the current workspace open in VS Code, your directory structure will look like the following:



```
LUA_PROGRAMMING
  .vscode
  conda_config
    xcanvas
    xeus-lua
    environment.yml
  node_modules
  notebooks
  scripts
    jupyter-lua-env.sh
  myst.yml
  package-lock.json
  package.json
```

Make sure you know where your `bash` is located. I am working in an Apple Silicon architecture and prefer to use `homebrew` to manage my packages rather than relying on the native MacOS installations of `python`, `bash`, etc. To install the latest version of `bash` just run:

```
brew install bash
```

Then locate your `.bashrc` file and add the `$BREW_PREFIX` to the `$PATH` variable with the following line:

```
export PATH="/opt/homebrew/bin:/opt/homebrew/sbin:$PATH"
```

Now, when you run the `which bash` command you should get the following output:

```
which bash
```

```
/opt/homebrew/bin/bash
```

Using a *shebang* or `#!`, we can put it in front of our path to ensure that our files are executable. This will will be the first line in both of our scripts.

We will use two scripts to get this job done. The first script will just create the virtual environment with its name (first parameter) and the Python version (second parameter).

While this is only one line, we are placing this in a different file because the execution ends after the environment is completed. This is where the second file comes in, allowing us to call the first script to create the environment, then using the rest of the script to build the Jupyter kernel.

Please find the complete scripts here:

- Script 1 (`01-create-env.sh`)
- Script 2 (`02-build-env.sh`)

Here is what the first file looks like:

```
#! /opt/homebrew/bin/bash
conda create -n $1 python=$2
```

If you are not familiar with `bash` syntax, `$1` represents the first parameter that is needed to run the file, whereas `$2` represents the second parameter.

For the second file, we will call `01-create-env.sh` and continue the kernel creation process. Here's what that looks like:

```
#! /opt/homebrew/bin/bash
# Run this script in the root directory as follows where <PROJECT_PREFIX>␣
↪is the absolute path to root directory or the output of pwd command:
# scripts/02-build-env.sh <PROJECT_PREFIX>

# Make configuration directory for
mkdir ./.config

```

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```
# Environment has been created. Now, we install the necessary packages in␣
↪it.
bash ./scripts/01-create-env.sh $1

# Source Miniconda so we can activate the env in the bash script.
source /opt/homebrew/Caskroom/miniconda/base/etc/profile.d/conda.sh

# Activate env and install ipykernel
conda activate jupyter-lua
conda install ipykernel

# Link environment to Jupyter
python -m ipykernel install --user --name=jupyter-lua

# Initialize node.js
npm init

# Install ijavascript kernel
npm install ijavascript
ijinstall

# Change to the conda_config directory for next few steps.
cd $1/.config

# Install xeus-lua kernel which has a dependency on xcanvas. This␣
↪dependency must be installed from source.
git clone git@github.com:jupyter-xeus/xcanvas.git
cd xcanvas && mkdir build && cd build
cmake -D CMAKE_INSTALL_PREFIX=$CONDA_PREFIX ..
make install

# Go back to the conda_config directory
cd $1/.config

# Install xeus-lua from source
git clone git@github.com:jupyter-xeus/xeus-lua.git
cd xeus-lua && mkdir build && cd build
cmake .. -D CMAKE_PREFIX_PATH=$CONDA_PREFIX -D CMAKE_INSTALL_PREFIX=
↪$CONDA_PREFIX -D CMAKE_INSTALL_LIBDIR=lib
```

First, we call `01-create-env.sh` with the parameters needed. This means that both files will using the same parameters. Once this is done, we must source `miniconda` such that we can activate the environment, use `conda` to install `ipykernel`, and link the environment to the kernel with the same name of the environment.

1.3 Running the Script

We can set permissions and run the script with the following where `<PROJECT_PREFIX>` is the `pwd`:

```
chmod -R 755 scripts
./scripts/02-build-env.sh <PROJECT_PREFIX>
```

This will create a new `conda` environment called `jupyter-lua`. Furthermore, as we saw in `02-build-env.sh`, it will also create a Jupyter kernel that is called `jupyter-lua`, which we can begin to use immediately after starting up Jupyter Notebooks.

CHAPTER

TWO

NEXT STEPS

We will return to these build scripts once we configure and build our own kernel with expanded features to better suit the project.

```
title: MyST Markdown Integration for Jupyter Notebooks
description: This notebook explores the conventions for yaml frontmatter␣
↪in MyST Formatted notebooks and some of the tool's other features.
date: 2024-01-04
```

```
%%html
<style>
    body {
        /* change --vscode-font-family if it's different on your system */
        --vscode-font-family: "lmroman17-regular"
    }
</style>
```

```
<IPython.core.display.HTML object>
```

CHAPTER

THREE

MYST MARKDOWN AND JUPYTER NOTEBOOK

MyST-NB is a Spinx and Docutils extension for compiling Jupyter Notebooks into high quality documentation formats.

This extension will allow us to mix Jupyter notebooks with text-based notebooks, Markdown, and RST documents. Using MyST flavored Markdown syntax –which extends CommonMark Markdown language including admonitions and additional syntax– we can author technical and scientific documentation through our regular Jupyter interface and render beautiful PDFs, MS Word Documents, LaTeX, and more.

I am really excited by using MyST as a potential substitute for my original `Pandoc` configuration project and want to turn this Jupyter setup into it's own separate build script so that it can be used added to future Jupyter environments.

:::{important} Objectives An important objective of this Jupyter Notebook is to understand the implementation of MyST and it's tools to generate better notebooks that can be converted to publish-quality products. :::

CHAPTER

FOUR

GETTING STARTED WITH MYST & SPHINX

CHAPTER

FIVE

FRONTMATTER

Frontmatter allows you to specify metadata and options about how your project should behave or render. Included in frontmatter are things like the document or project `title`, what `thumbnail` to use for sit or content previews, `authors` that contributed to the work, and scientific identifiers like a `doi`. Adding frontmatter ensures that these properties are available to downstream tools or build processes like building **Scientific PDFs**.

5.1 Where to set frontmatter

Frontmatter can be set in a markdown (`md`) or notebook (`ipynb`) file (described as a "page" below) or in the `project:` section of a `myst.yml` file. When project frontmatter is set in a `myst.yml` file, those settings will be applied to all content in that project (apart from "page only" fields).

5.1.1 In a MyST markdown file

A frontmatter section can be added at the top of any `md` file using `---` delimiters.

```yaml
title: My First Article
date: 2024-01-04
authors:
    - Nyki Anderson
      affiliations:
        - University of Europe
```

5.1.2 In a Jupyter Notebook

Frontmatter can be added to the first cell of a Jupyter Notebook, that cell should be a Markdown cell and use `---` delimiters as above.

> **Hint!** Install JupyterLab Myst To have properly formatted frontmatter, you can install the `jupyterlab-myst` plugin for Jupyter.
>
> `pip install jupyterlab_myst`
>
> Without the extension installed, remember to format the contents of the section as valid `yaml` even though when rendered, the cell will not look well formatted in your notebook.

5.1.3 In a `myst.yml` file

Frontmatter fields can be added directly to any `project:` section within a `myst.yml` file. If your root `myst.yml` file only contains a `site:` section, and you want to add frontmatter, add a `project:` section at the top level and add the fields there, e.g.,

```yaml
myst: v1
site:
project:
    license: CC-BY-4.0
    open_access: true
```

5.2 Available frontmatter fields

The following table lists the available frontmatter fields, a brief description and a note on how the field behaves depending on whether it is set on a page or at the project level. Where a field itself is an object with sub-fields, see the relevant description on the page below.

- `title` - a string (page & project)
- `description` - a string (page & project)
- `short_title` - a string (page & project)
- `name` - a string (page & project)
- `tags` - a list of strings (page only)
- `thumbnail` - a link to a local or remote image (page only)
- `subtitle` - a string (page only)
- `date` - a valid date (page can override project)

- `authors` - a list of author objects (page can override project)
- `affiliations` - a list of affiliation objects (page can override project)
- `doi` - a valid DOI, either URL or id (page can override project)
- `arxiv` - a valid arXiv reference, either URL or id (page can override project)
- `open_access` - boolean (page can override project)
- `license` - a license object or a string (page can override project)
- `funding` - a funding object (page can override project)
- `github` - a valid GitHub URL or `owner/reponame` (page can override project)
- `binder` any valid URL (page can override project)
- `subject` - a string (page can override project)
- `venue` - a venue object (page can override project)
- `biblio` - a biblio object with various fields (page can override project)
- `math` - a dictionary of math macros (page can override project)
- `abbreviations` - a dictionary of abbreviations in the project (page can override project)
- `parts` - a dictionary of arbitrary content parts, not part of the main article, for example `abstract`, `data_availability` (page only)
- `options` - a dictionary of arbitrary options validated and consumed by templates, for example, during site or PDF build (page can override project)

5.3 Field Behavior

Frontmatter can be attached to a "page", meaning a local `.md` or `.ipynb` or a "project". However, individual frontmatter fields are not uniformly available at both levels, and certain behavior of certain fields are different between project and page levels. There are three field behaviors to be aware of:

- `page & project` : the field is available on both th epage & project but they are independent
- `page only` : the field is only available on pages, and not present on projects and it will be ignored if set there.
- `page can override project` : the field is available on both page & project but the value of the field on the page will override any set of the project. Note that the page field must be omitted or undefined, for the project value to be used, value of `null` (or `[]` in the case of `authors`) will still override the project value but clear the field for that page.

5.4 Thumbnail & Banner

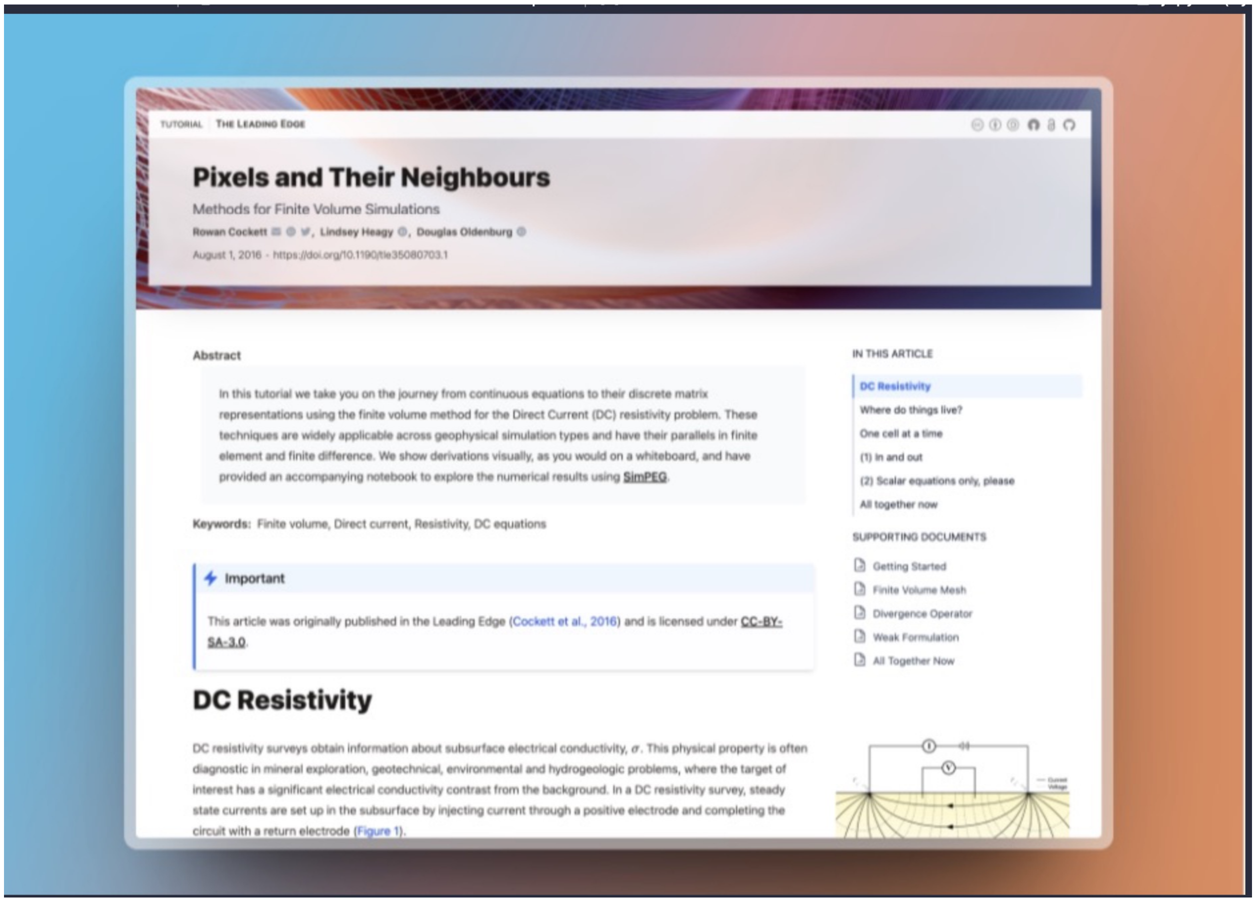
The thumbnail is used in previews for your site in applications like Twitter, Slack, or any other link preview service. This should, by convention, be included in a `thumbnails` folder next to your content. You can also explicitly set this field to any other image on your local file system or a remote URL to an image. This image will get copied over to your public folder and optimized when you build your project.

```yaml
thumbnail: thumbnails/myThumbnail.png
```

If you do not specify an image the first image in the content of a page will be selected. If you explicitly do not want an image, set `thumbnail` to `null`.

You can also set a banner image which will show up in certain themes, for example, the `article-theme`:

```yaml
banner: banner.png
```



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Pixels and Their Neighbours

Methods for Finite Volume Simulations

Rowan Cockett, Lindsey Heagy, Douglas Oldenburg

August 1, 2016 - https://doi.org/10.1190/tle35080703.1

Abstract

In this tutorial we take you on the journey from continuous equations to their discrete matrix representations using the finite volume method for the Direct Current (DC) resistivity problem. These techniques are widely applicable across geophysical simulation types and have their parallels in finite element and finite difference. We show derivations visually, as you would on a whiteboard, and have provided an accompanying notebook to explore the numerical results using SimPEG.

Keywords: Finite volume, Direct current, Resistivity, DC equations

Important

This article was originally published in the Leading Edge (Cockett et al., 2016) and is licensed under CC-BY-SA-3.0.

DC Resistivity

DC resistivity surveys obtain information about subsurface electrical conductivity, σ. This physical property is often diagnostic in mineral exploration, geotechnical, environmental and hydrogeologic problems, where the target of interest has a significant electrical conductivity contrast from the background. In a DC resistivity survey, steady state currents are set up in the subsurface by injecting current through a positive electrode and completing the circuit with a return electrode (Figure 1).

IN THIS ARTICLE

DC Resistivity
Where do things live?
One cell at a time
(1) In and out
(2) Scalar equations only, please
All together now

SUPPORTING DOCUMENTS

Getting Started
Finite Volume Mesh
Divergence Operator
Weak Formulation
All Together Now

5.5 Authors

The `authors` field is a list of `author` objects. Available fields in the author object are:

- `name` : a string OR CSL-JSON author object - the author's full name; if a string, this will be parsed automatically. Otherwise, the object may contain `given`, `surname`, `non_dropping_particle`, `dropping_particle`, `suffix`, and full name `literal`.
- `orcid` : a string - a valid ORCID identifier with or without the URL.
- `corresponding` : boolean - flags any corresponding authors, you must include an `email` if true.
- `url` : a string - website or homepage of the author.
- `roles` : a list of strings - must be valid **CRediT Contributor Roles**.

```
authors:
    - name: Nyki Anderson
      roles:
        - Conceptualization
        - Data curation
        - Validation
```

CRediT Roles

There are 14 official contributor roles that are in the NISO CRediT Role standard. In addition to British english, incorrect case or punctuation, there are also a number of aliases that can be used for various roles.

- Conceptualization (alias: conceptualisation)
- Data curation
- Formal analysis (alias: analysis)
- Funding acquisition
- Investigation
- Methodology
- Project administration (alias: administration)
- Resources
- Software
- Supervision
- Validation
- Visualization (alias: visualisation)

  - Writing - original draft (alias: writing)
  - Writing - review & editing (alias: editing, review)

- `affiliations` : a list of strings that identify or create an affiliation or a full `Affiliation` object, for example:

```
authors:
    - name: Nyki Anderson
      affiliations:
        - id: ubc
          institution: University of British Columbia
          ror: 034rmrcq20
          department: Earth, Ocean and Atmospheric Sciences
        - ACME Inc
    - name: Julian Todman
      affiliation: ubc
```

See Affiliations for more information on how to concisely write affiliations.

- `equal-contributor` : a boolean, indicates that the author is an equal contributor.
- `deceased` : a boolean, indicates that the author is a deceased.
- `twitter` : a twitter username.
- `github` : a GitHub username.
- `note` : a string, a freeform field to indicate additional information about the author, for example, acknowledgments or specific correspondence information.
- `phone` : a phone number, e.g., (301) 754 - 5766.
- `fax` : for people who still use these machines.

5.6 Affiliations

You can create an affiliation directly by adding it to an author, and it can be as simple as a single string.

```
authors:
    - name: Nyki Anderson
      affiliation: University of British Columbia
```

You can also add much more information to any affiliation, such as a ROR, ISNI, or an address. A very complete affiliations list for an author at the University of British Columbia is:

```yaml
authors:
    - name: Nyki Anderson
      affiliations:
        - id: ubc
          institution: University of British Columbia
          ror: https://ror.org/03rmrcq20
          isni: 0000 0001 2288 9830
          department: Department of Earth, Ocean and Atmospheric Sciences
          address: 2020 - 2207 Main Mall
          city: Vancouver
          region: British Columbia
          country: Canada
          postal_code: V6T 1Z4
          phone: 604 822 2449
    - name: Julian Todman
      affiliation: ubc
```

Notice how you can use an `id` to avoid writing this out for every coauthor. Additionally, if the affiliation is a single string and contains a semi-colon `;` it will be treated as a list. The affiliations can also be added to your `project` frontmatter in your `myst.yml` and used across any document i the project.

```yaml
# article.md
title: My Article
authors:
  - name: Nyki Anderson
    affiliation: ubc
  - name: Julian Todman
    affiliations: ubc; stanford
```

```yaml
# myst.yml
affiliations:
  - id: ubc
    institution: University of British Columbia
    ror: https://ror.org/03rmrcq20
    isni: 0000 0001 2288 9830
    department: Department of Earth, Ocean and Atmospheric Sciences
    address: 2020 - 2207 Main Mall
    city: Vancouver
    region: British Columbia
    country: Canada
    postal_code: V6T 1Z4
    phone: 604 822 2449
  - id: stanford
```

If you use a string that is not recognized as an already defined affiliation in the project or article frontmatter, an affiliation will be created automatically and normalized so that it can be referenced:

```yaml
# Written Frontmatter
authors:
  - name: Marissa Myst
    affiliations:
      - id: ubc
        institution: University of British Columbia
        ror: 03rmrcq20
        department: Earth, Ocean and Atmospheric Sciences
      - ACME Inc
  - name: Miles Mysterson
    affiliation: ubc
```

```yaml
# Normalized
authors:
  - name: Marissa Myst
    affiliations: ['ubc', 'ACME Inc']
  - name: Miles Mysterson
    affiliations: ['ubc']
affiliations:
  - id: ubc
    institution: University of British Columbia
    ror: https://ror.org/03rmrcq20
    department: Earth, Ocean and Atmospheric Sciences
  - id: ACME Inc
    name: ACME Inc
```

- `id` : a string - local identifier that can be used to easily reference a repeated affiliation.
- `name` : a string - the affiliation name. Either `name` or `institution` is required.
- `institution` : a string - Name of an institution or organization (for example, a university or corporation). If your research group has a name, you can use both `name` and `institution`, however, at least one of these is required.
- `department` : a string - the affiliation department (e.g., Chemistry).
- `doi`, `ror`, `isni`, `ringgold` : identifiers for the affiliation (DOI, ROR, ISNI, and Ringgold). We suggest using https://ror.org if possible to search for your institution.

```yaml
affiliations:
  - name: Boston University
    ringgold: 1846
    isni: 0000 0004 1936 7558
```

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```
    ror: 05qwgg493
    doi: 10.13039/100018578
```

- `email` : a string - email of the affiliation, required if `corresponding` is `true`.
- `address, address`, `city`, `state`, `postal code`, and `country` : affiliation address information, in place of `state` you can use `province` or `region`.
- `url` : a string - website or homepage of the affiliation (`website` is an alias).
- `phone` : a phone number, e.g., (301) 754 5766.
- `fax` : A fax number for the affiliation.
- `collaboration` : a boolean - indicate that the affiliation is a collaboration, for example, “MyST Contributors” can be both an affiliation and a listed author. This is used in certain templates as well as in **JATS**.

5.7 Date

The date field is a string and should conform to a valid Javascript data format. Examples of acceptable date formats are:

```
2021-12-14T10:43:51.777Z - an ISO 8601 calendar date extended format, or
14 Dec 2021
14 December 2021
2021, December 14
2021 December 14
12/14/2021 - MM/DD/YYYY
12-14-2021 - MM-DD-YYYY
2022/12/14 - YYYY/MM/DD
2022-12-14 - YYYY-MM-DD
```

Where the latter example in that list are valid **IETF-timestamps**.

5.8 Licenses

This field can be set to a string value directly or to a License object.

Available fields in the License object are `content` and `code` allowing licenses to be set separately for these two forms of content, as often different subsets of licenses are applicable to each. If you only wish to apply a single license to your page or project use the string form rather than an object.

String values for licenses should be a valid “Identifier” string from the SPDX License List. Identifiers for well-known licenses are easily recognizable (e.g., `MIT` or `BSD`) and MyST will attempt to infer the specific identifier if an ambiguous license is specified (e.g., `GPL` will be interpreted as `GPL-3.0+` and a warning raised letting you know of this interpretation). Some common licenses are:

```
# Common Content Licenses
CC-BY-4.0
CC-BY-SA-4.0
CC-BY-N-SA-4.0
CC0-1.0
```

```
# Common Code Licenses
MIT
BSD
GPL-3.0+
Apache-2.0
LGPL-3.0-or-later
AGPL
```

By using the correct SPDX Identifier, your website will automatically use the appropriate icon for the license and link to the license definition.

5.9 Funding

Funding frontmatter is able to contain multiple funding and open access statements, as well as award info.

It may be as simple as a single funding statement:

```
funding: This work was supported by University.
```

Funding may also specify award id, name, sources (`affiliation object` or `reference`), investigators (`contributor objects` or `references`), and recipients (`contributor objects` or `references`).

```
authors:
  - id: auth0
    name: Jane Doe
funding:
  statement: This work was supported by University.
  id: award-id-000
  name: My Award
```

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```
  sources:
    - name: University
  investigators:
    - name: John Doe
  recipients:
    - auth0
```

Multiple funding objects with multiple awards are also possible:

```
authors:
  - id: auth0
    name: Jane Doe
funding:
  - statement: This work was supported by University.
    awards:
      - id: award-id-000
        name: My First Award
        sources:
          - name: University
        investigators:
          - name: John Doe
        recipients:
          - auth0
      - id: award-id-001
        name: My Second Award
        sources:
          - name: University
        investigators:
          - name: John Doe
        recipients:
          - auth0
  - statement: Open access was supported by Consortium.
    open_access: Users are allowed to reproduce without prior permission
    awards:
      - id: open-award-999
        sources:
          - name: Consortium
```

5.10 Venue

The term `venue` is borrowed from the **OpenAlex** API definition:

Venues are where works are hosted.

Available fields in the `venue` object are `title` and `url`.

Some typical `venue` values may be:

```yaml
venue:
  title: Journal of Geophysics
  url: https://journal.geophysicsjournal.com
```

```yaml
venue:
  title: EuroSciPy 2022
  url: https://www.euroscipy.org/2022
```

5.11 Biblio

The term `biblio` is borrowed from the **OpenAlex** API definition:

Old-timey bibliographic info for this work. This is mostly useful only in citation/reference contexts. These are all strings because sometimes you'll get fun values like "Spring" and "Inside cover."

Available fields in the `biblio` object are `volumne`, `issue`, `first_page` and `last_page`.

Some example `biblio` values may be:

```yaml
biblio:
  volume: '42'
  issue: '3'
  first_page: '1' # can be a number or string
  last_page: '99' # can be a number or string
```

```yaml
biblio:
  volume: '2022'
  issue: Winter
  first_page: Inside cover # can be a number or string
```

CHAPTER SIX

SETTINGS

The `settings` field in the project or page frontmatter allows you to change how the parsing, transforms, plugins, or other behaviors of mystmd.

6.1 Available settings fields

- `output_stderr` : Remove, warn, or error on `stderr` outputs (e.g., `DeprecationWarnings`, `RuntimeWarnings`).
  - `show` : (default) : show all `stderr` (unless a `remove-stderr` tag is present on the cell).
  - `remove` : remove all `stderr` outputs.
  - `remove-warn` or `remove-error` : remove all `stderr`, and log a warning or error.
  - `warn` or "error" : log a warning or error if a `stderr` is found.
- `output_stdout` : Remove, warn or error on `stdout` outputs. (e.g., long text outputs, like text-based progress bars).
  - `show` : (default) : show all `stdout` (unless a `remove-stdout` tag is present on the cell).
  - `remove-warn` or `remove-error` : remove all `stdout`, and log a warning or error.
  - `warn` or "error" : log a warning or error if a `stdout` is found.
- `output_matplotlib_strings` : Remove, warn, or error on matplotlib strings outputs. (e.g., <Figure size 720x576 with 1 Axes> or Text(0.5, 0.98, 'Test 1')). These can also be suppressed by ending your cell content with a semicolon in Jupyter Notebooks. The default is to remove these and warn (`remove-warn`).
  - `show` : show al matplotlib strings in outputs.
  - `remove` : remove all matplotlib strings in outputs
  - `remove-warn` : (default) or `remove-error` : remove all matplotlib strings in outputs, and log a warning or error.

  - `warn` or “error” : log a warning or error if matplotlib strings in outputs.

CHAPTER

SEVEN

MORE FROM MYST MARKDOWN

Most of this Notebook has been focused on the use of frontmatter to enrich the quality and dynamism of our projects. But from skimming through the extensive documentation, it is clear that MyST Markdown Tools might have more value than just allowing richer metadata in Jupyter Notebooks.

According to the MyST Markdown homepage, their tools are designed to revolutionize scientific communication in its various forms. Labeling itself an "authoring framework," MyST products handle blogs, online books, scientific papers, reports, and journal articles.

7.1 Key Features

- **Rabbit-hole links** allow you to get information to your reader as fast as possible and they can deep-dive all the way to computations, code, and interactive figures.
- **Live graphs** can be embedded directly in your documentation or articles with computation backed by Jupyter –running locally, on Binder, or directly in your browser.
- **JupyterLab support** for MyST comes with inline computations, support for `ipywidgets`, matplotlib sparklines, editable task-lists, rich frontmatter (as we know already), and beautiful typography and other elements like dropdowns, grids and cards.
- **Export to PDF** is easy and they support hundreds of different journals out of the box, see myst-templates. You can also export to Microsoft Word or JATS, which is used in scientific publishing.

7.2 Project Goals

MyST is part of the Executable Books organization, which is a community driven project to improve scientific communication, including integrations into Jupyter Notebooks and computational results.

7.2.1 Built for Science

Extend Markdown with equations, cross-references, citations, and export to preprint or rich, interactive website or book.

7.2.2 Dynamic Documents

Make your pages interactive by connecting to custom JupyterHubs, public Binders, or even Python directly in your browser.

7.2.3 Fast & Accessible

Publish next-generation articles and books that are beautifully designed, without compromising on accessibility or performance.

7.2.4 Technical Goals

- `mystmd` is a Javascript parser and command line tool for working with MyST Markdown.
- Parse MyST into a standardized **AST**, that follows the MyST Spec.
- Translate and render MyST into:
  - Modern **interactive websites**, using React.
  - PDFs and LaTeX documents, with specific templates for over 400 journals.
  - Microsoft Word **export**.
- Provide functionality for *cross-referencing*, *external structured links*, and *scientific citations*.

7.3 Installing the MyST Markdown CLI

`mystmd` is a command line interface that provides modern tooling for technical writing, reproducible science, and creating scientific & technical websites. To get started, install `mystmd`.

7.3.1 Prerequisites - Install Node

You should have these programs installed already from our last Notebook:

- `Node.js` version >=18.0.0
- `npm` version >=7.0.0
- A code and notebook editor (`VS Code` and `Jupyter Lab` for notebooks).

7.3.2 Install the MyST CLI

Install node https://nodejs.org/ or through conda.

```
conda install -c conda-forge 'nodejs>=20,<21'
```

```
zsh:1: 20, not found

Note: you may need to restart the kernel to use updated packages.
```

Then install `mystmd`:

```
conda install mystmd -c conda-forge
```

```
Channels:
 - conda-forge
 - defaults
Platform: osx-arm64
Collecting package metadata (repodata.json): done
Solving environment: done

# All requested packages already installed.


Note: you may need to restart the kernel to use updated packages.
```

7.4 Circle Back at a Later Date

All of the promising features of MyST have certainly piqued my interests though much of the functionality is beyond the scope of the current state of my many projects. I will certainly be returning to this documentation when I begin publishing my Ancestry Research findings and as academic or professional opportunities come my way.

For now, we will focus our attention on producing thorough metadata through page-level directives and potentially project level-directives as we become more comfortable with the Jupyter Notebook system as a whole.

Let's run back through this and the previous Notebook to input some quick metadata and move on to the next topic.

CHAPTER

EIGHT

CONFIGURING SPHINX TO RENDER HTML & PDF VERSIONS OF JUPYTER NOTEBOOKS

Objectives

The objectives for this notebook are as follows:

- Integrate MyST Markdown and Sphinx documentation tools to produce a beautifully rendered HTML page on GitHub pages as well as a nicely formatted LaTeX-generated PDF.
- Understand how to properly configure and add metadata to the document as a whole as well as at the notebook-level.
- Begin to customize the entire pipeline so that it is both automated and efficient.

8.1 Prerequisites

It is highly recommended that you use the `conda` environment scripts found in the `scripts/` folder. They can be run from the root directory like this:

```
chmod -R 755 scripts/
./scripts/02-build-env.sh <PATH_TO_ROOT>
```

Note

Note that the `<PATH_TO_ROOT>` is passed here as an argument to the script, therefore it must be absolute. You can find this variable by simple typing `pwd` from the root directory of the project.

Close all terminals and start a fresh session. To be certain that the environment you just built is your active `conda` environment:

```
conda activate jupyter
```

You can now navigate to your project root folder and issue the command to open with VS Code:

```
code Jupyter-Notebooks-MyST-and-Sphinx/
```

A fresh instance of your project will open in VS Code. Now enter the command pallet `CMD-Shift-P` and select `Python: Select Interpreter`. Choose the version with the name of your `conda` environment, it should be named `jupyter`.

Next create a `docs/` folder in the root directory and inside of it, create a `notebooks/` folder. This will be where we keep all of our notebooks.

Start your first Jupyter notebook by creating a file with the extension `.ipynb` and open that file. Create a new Markdown cell and type some dummy info. We will need content to test our configuration of Sphinx and the other tools.

Now we can begin the deep-dive into the Sphinx and MyST-NB configuration process.

8.2 Getting Started with Sphinx

Documentation

For the full Sphinx Documentation visit sphinx-doc.org. There are a lot of options… Sphinx is highly complex so I have tried to distill it down in these notebooks for you. Still, the documentation will provide all configuration options available for a more custom experience.

I used a wonderful OBM Research Group tutorial[1] to configure most of Sphinx, though I tried my hand manually and had my fair share of trial and error.

```
title: Build Custom Kernel
description: This Notebook will detail how to implement a customer kernel␣
↪with support for IPython which Xeus-Lua does not do out-of-the-box.
date: 2024-01-04
jupytext:
    formats: md:myst
    text-representation
```

[1] Tutorial: Sphinx environment with Conda

```
%%html
<style>
    body {
        --vscode-font-family: "lmroman17-regular"
    }
</style>
```

```
<IPython.core.display.HTML object>
```

CHAPTER

NINE

BUILDING A CUSTOM JUPYTER NOTEBOOK KERNEL

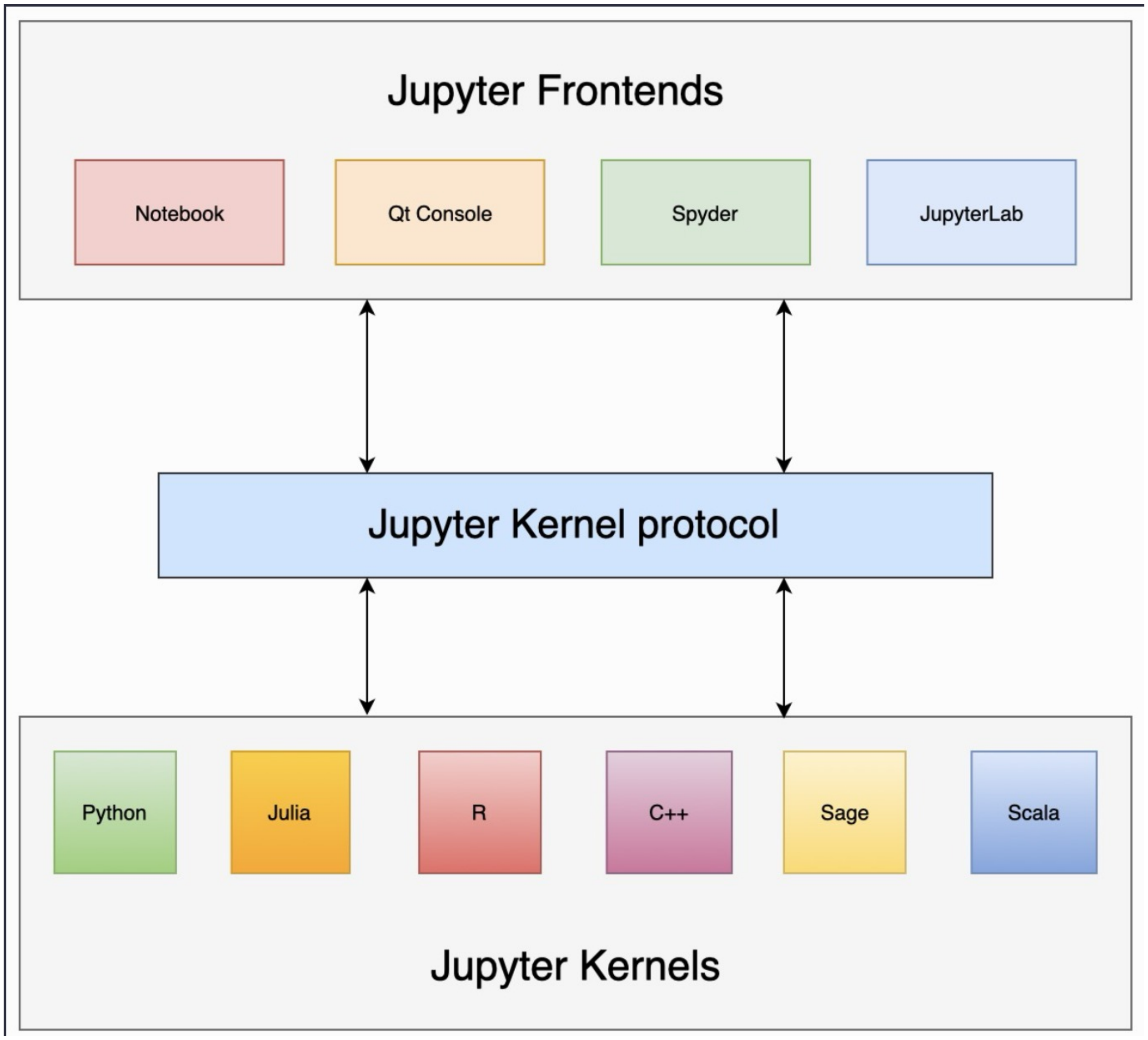
I found when starting the Lua Programming Udemy course that the stock `xeus-lua` kernel was not dynamic enough to allow so-called *magic* commands offered by the IPython Kernel. Specifically, I could not run the `lua` code as files that receive user input.

In reaction –and at risk of becoming too granular– I am taking this opportunity to learn how to build my own custom Jupyter kernel.

:::{important} Objectives The objective of this exercise is to build a custom `lua` kernel that allows for the use of magic `shell` commands within the `lua` code cells. :::

9.1 Using `xeus` to Author Custom Kernels

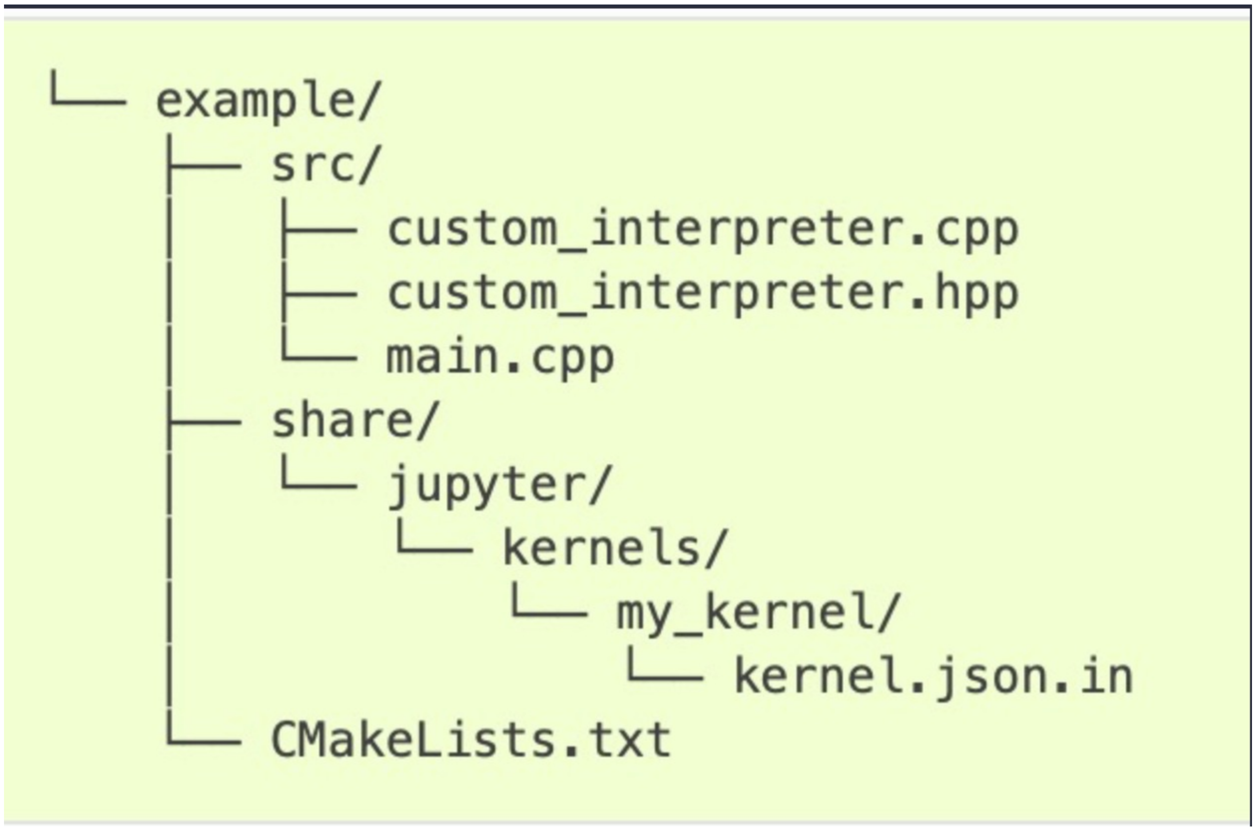
`xeus` enables custom kernel authors to implement Jupyter kernels more easily. It takes the burden of implementing the Jupyter Kernel protocol so developers can focus on implementing the interpreter part of the kernel.



9.2 Implementing a Kernel

In most of the cases, the base kernel implementation is enough, and creating a kernel only means implementing the interpreter part.

The structure of our project should at least look like the following:



```
└── example/
    ├── src/
    │   ├── custom_interpreter.cpp
    │   ├── custom_interpreter.hpp
    │   └── main.cpp
    ├── share/
    │   └── jupyter/
    │       └── kernels/
    │           └── my_kernel/
    │               └── kernel.json.in
    └── CMakeLists.txt
```

CHAPTER TEN

INDICES AND TABLES

- genindex
- modindex
- search