template

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I. JUPYTER NOTEBOOK TEMPLATE

This is a template file for scientific projects.

The project leans heavilly on the excellent review of Julius Schultz and uses the template from Michael Goerz.

Jupyter notebooks are great as they allow you to write code together with text.

A. Simple output

For example below is the function

$$A = \sum_{ij} \delta_{i,j}$$

where $\delta_{i,j}$ is the Kronecker delta function.

Citations also work by the way [1] [2].

```
[[1. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 [0. 1. 0. 0. 0. 0. 0. 0. 0. 0.]
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 0.]
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0.]
 [0. 0. 0. 0. 0. 1. 0. 0. 0. 0.]
 [0. 0. 0. 0. 0. 0. 1. 0. 0. 0.]
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0.]
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0.]
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]]
```

B. MD Analysis

This output doesn't show in pdf format. But is very handy in html exports.

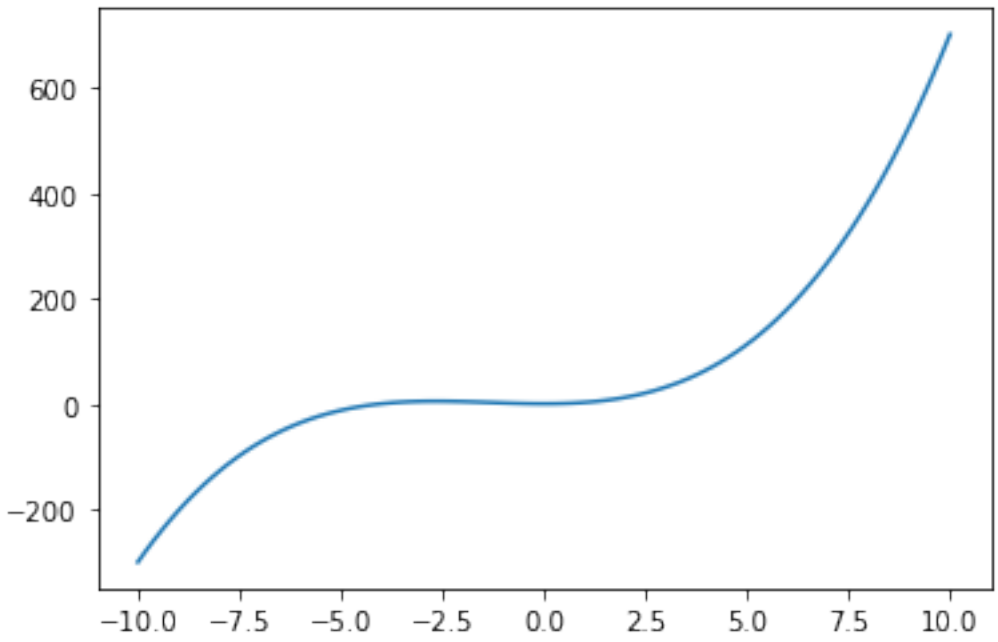
a. MAKE SURE TO SAVE THE WIDGET STATE!!! To do this go to `Widgets-> Save Notebook Widget State`

```
/home/marick/anaconda3/lib/python3.8/site-
packages/MDAnalysis/topology/PDBParser.py:330: UserWarning: Element␣
 ↪information is
absent or missing for a few atoms. Elements attributes will not be␣
 ↪populated.
  warnings.warn("Element information is absent or missing for a few "
```

```
NGLWidget(max_frame=50)
```

C. Matplotlib

And a matplotlib example



D. References

[1] T. l. C. Jansen and J. Knoester, Nonadiabatic effects in the two-dimensional infrared spectra of peptides: application to alanine dipeptide, The Journal of Physical Chemistry B **110**, 22910 (2006).

[2] N. J. Hestand and F. C. Spano, Expanded theory of h- and j-molecular aggregates: The effects of vibronic coupling and intermolecular charge transfer, Chemical Reviews **118**, 7069 (2018).