UConnRCMPy: Python-based Data Analysis for Rapid Compression Machines

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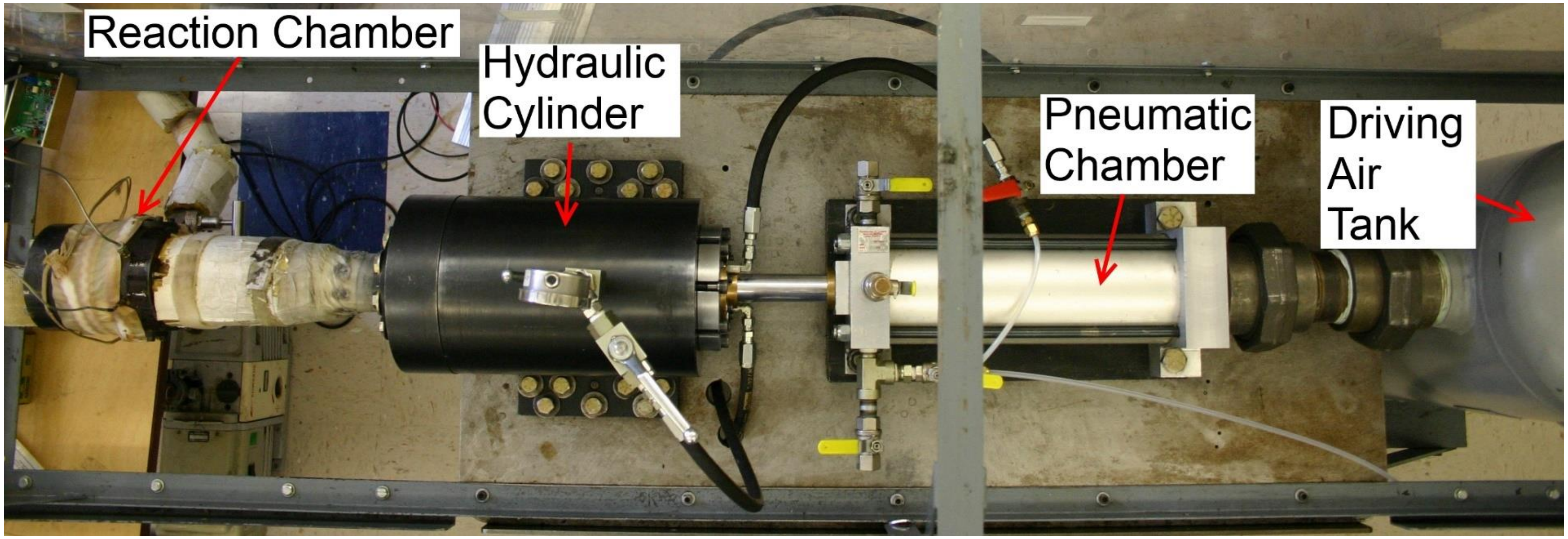
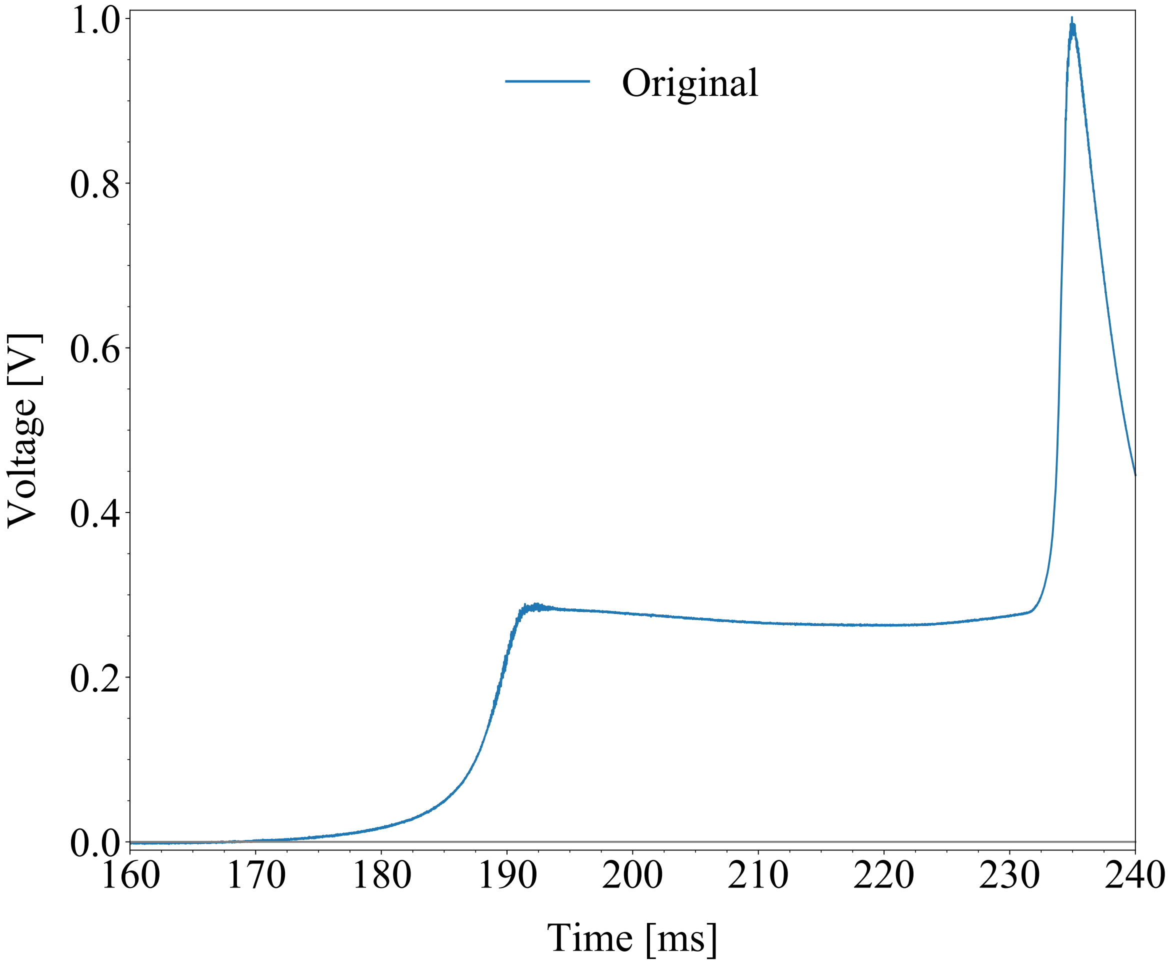
Rapid Compression Machines

- High pressure and low temperature conditions
- Minimize effects of fluid mechanics and inhomogeneity
- 25+ RCMs in use around the world

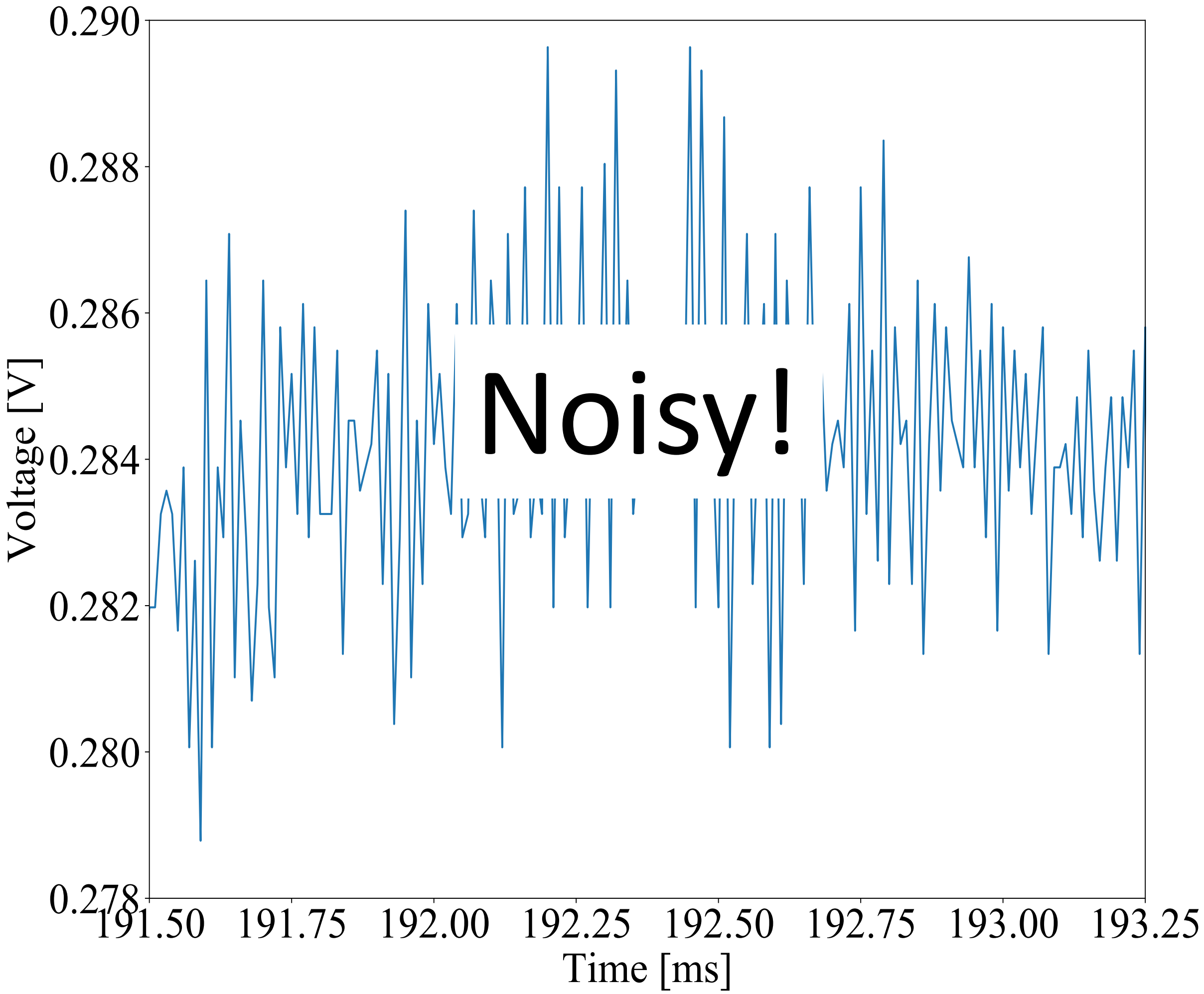


What do we measure?



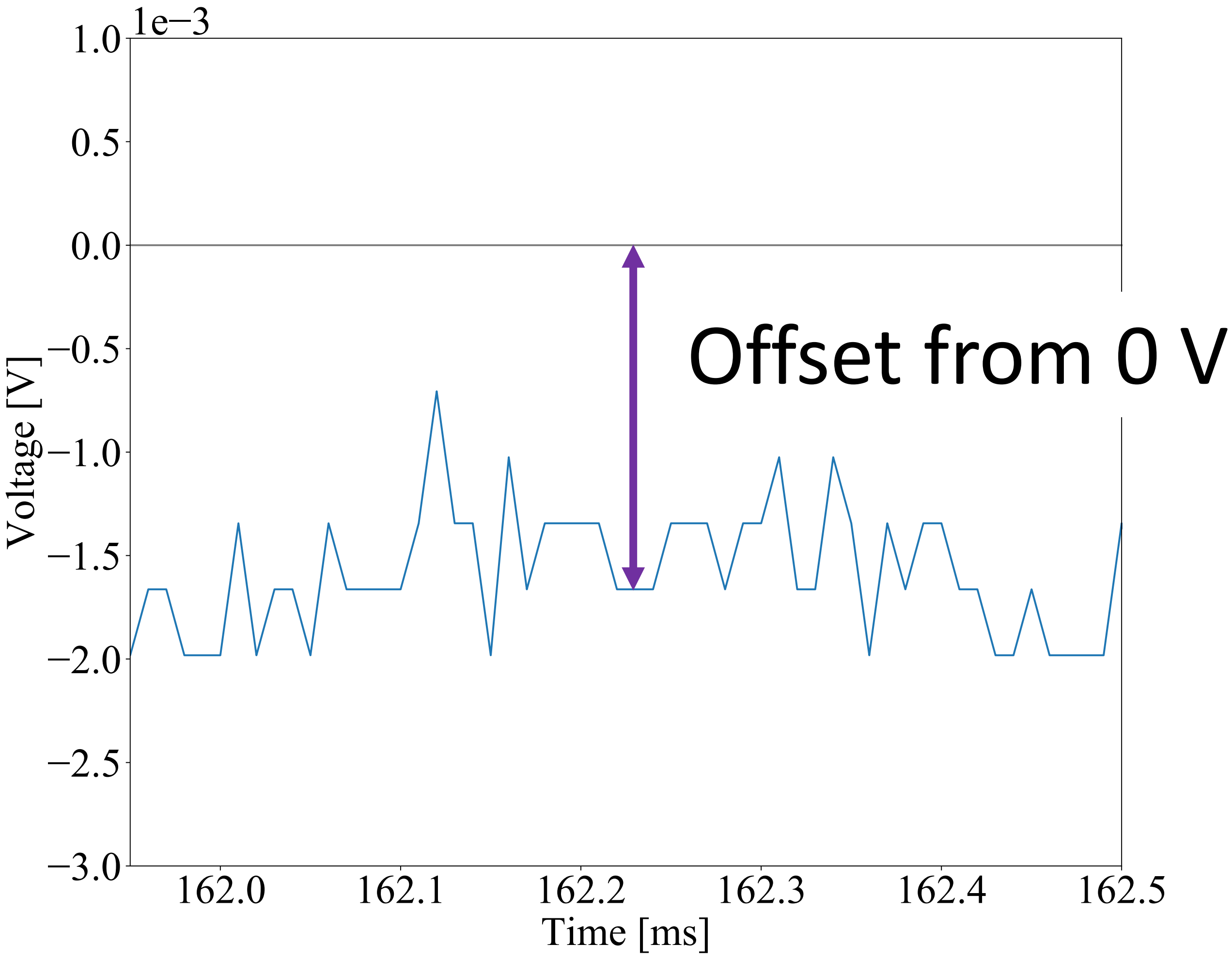
A piezo-transducer outputs a charge signal as pressure changes→ converted to voltage, recorded by computer

Voltage Trace



Noisy!

Voltage Trace



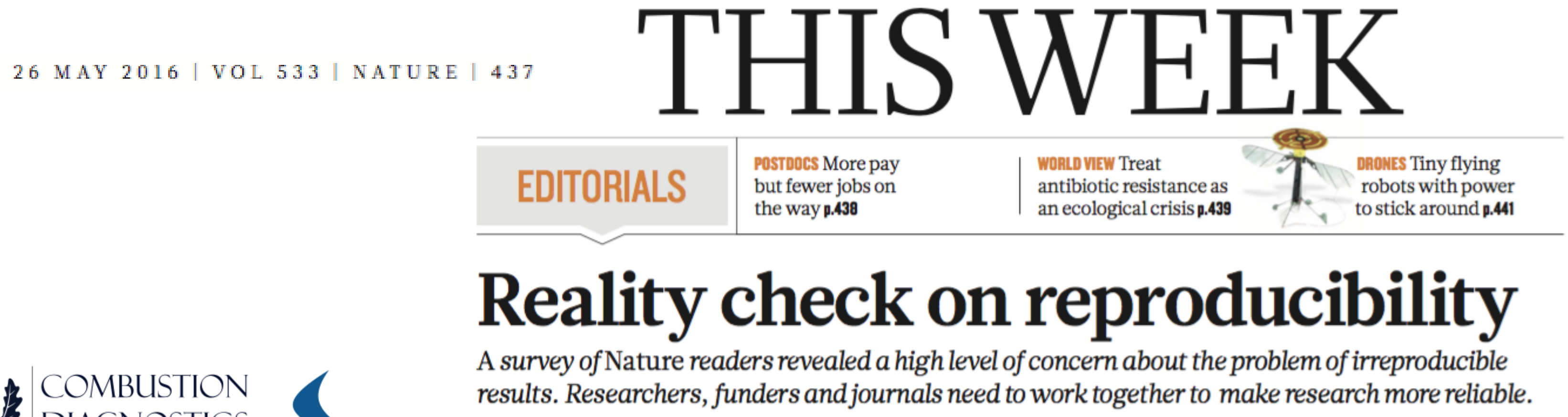
Offset from 0 V

What do we measure?

- A dynamic pressure transducer produces a charge output that is converted to a 0–10 V output
- Nominally, the initial voltage before compression is 0 V
- Ideally, the signal will be free of noise
- **The voltage must be processed to compute the pressure, temperature, and ignition delay**

~~Problems~~ Engineering Opportunities

- The signal is noisy → Error in P_C
- There is an offset in the initial voltage → Error in P_0, T_C
- There are 25+ RCMs in the world, and everyone uses a different processing procedure
- Reproducibility is important!



26 MAY 2016 | VOL 533 | NATURE | 437

THIS WEEK

EDITORIALS

POSTDOCS More pay but fewer jobs on the way p.438

WORLD VIEW Treat antibiotic resistance as an ecological crisis p.439

DRONES Tiny flying robots with power to stick around p.441

Reality check on reproducibility

A survey of Nature readers revealed a high level of concern about the problem of irreproducible results. Researchers, funders and journals need to work together to make research more reliable.

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Let’s use Python to write a data analysis framework with the following goals:

1. Reproducible analysis across researchers
2. Documented design choices for filter criteria, etc.
3. Citable, open-source publication of code

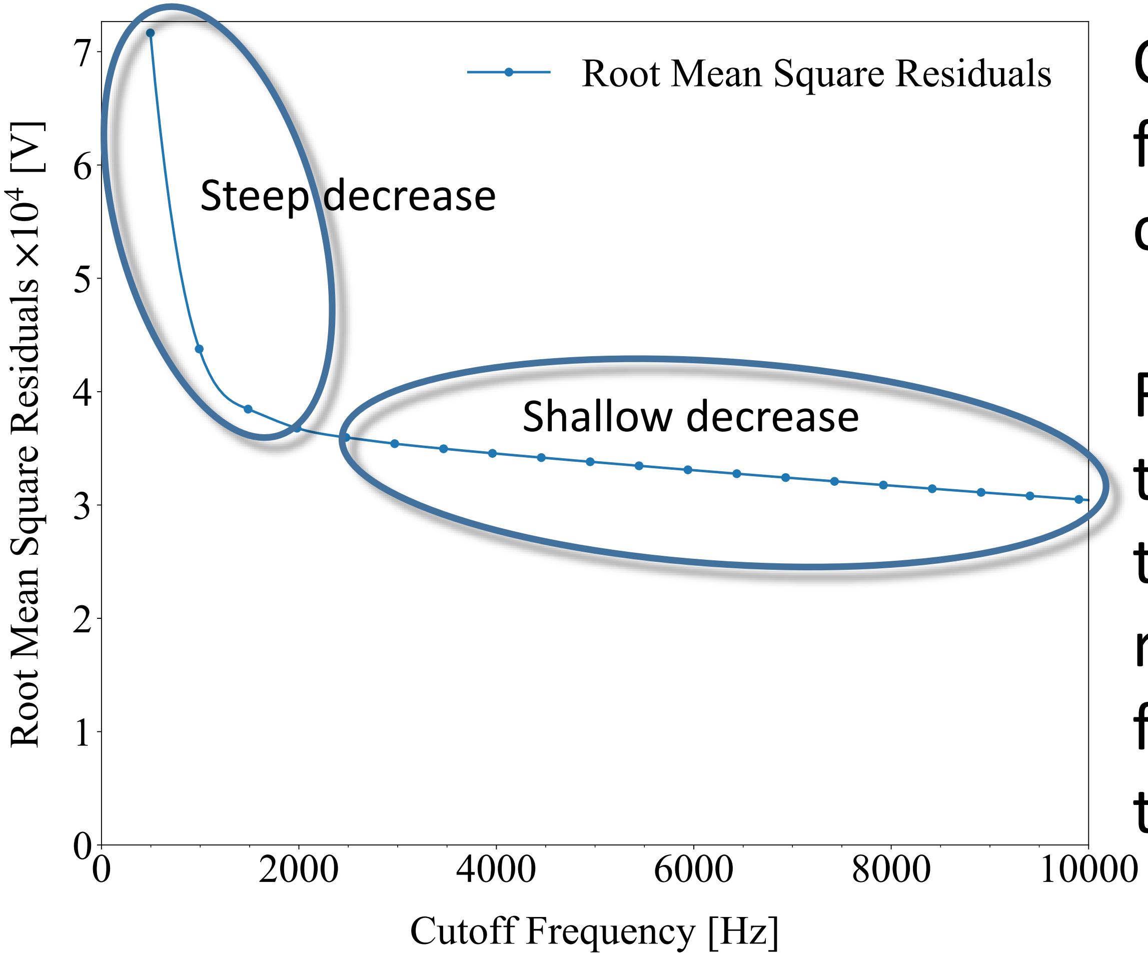
UConnRCMPy

https://github.com/bryanwweber/UConnRCMPy

Features of UConnRCMPy

- Low-pass filtering the raw voltage trace
    - Automatic filter cutoff frequency selection
- Converting the voltage trace into a pressure trace
- Processing the pressure trace to determine
    - ignition delay(s)
    - machine-specific effects on the experiment
- Calculating T_C from experiments

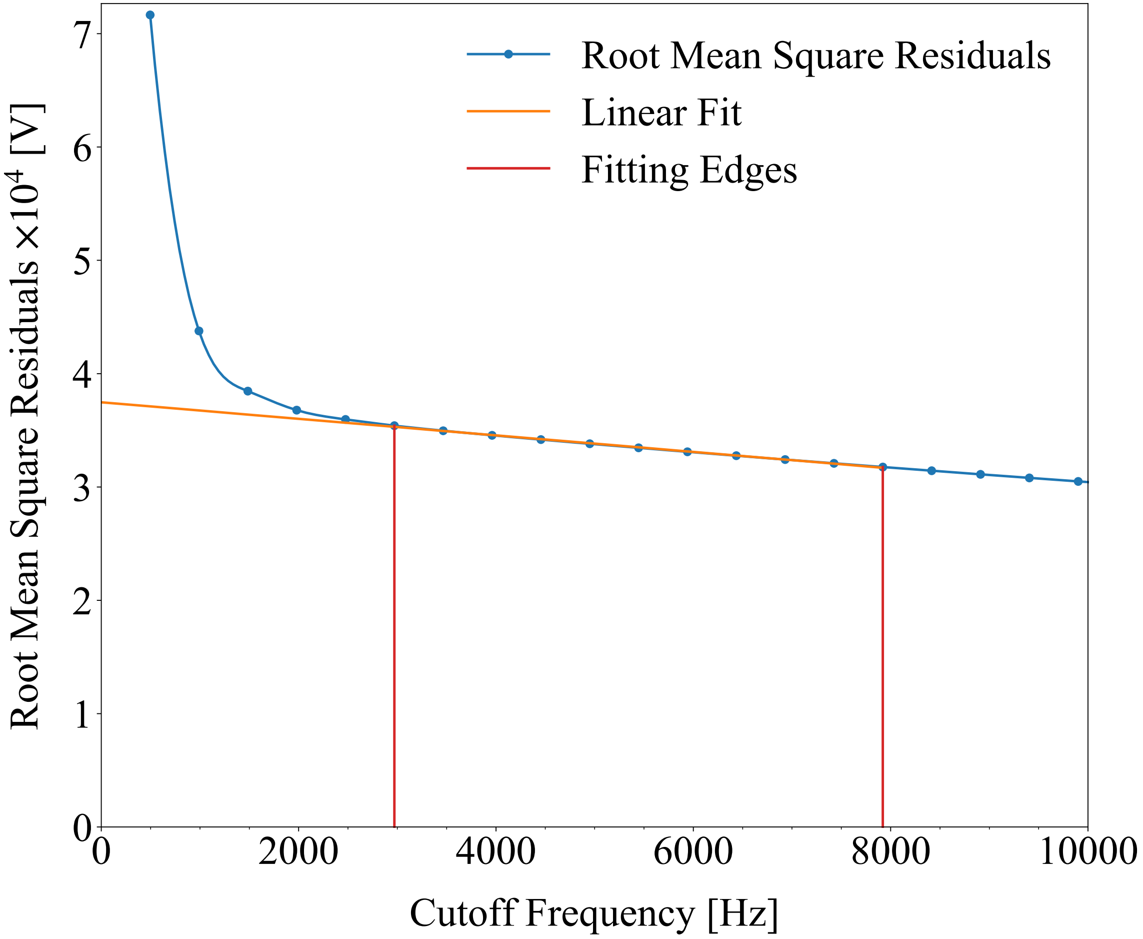
Filter Cutoff Frequency affects residuals



Construct low-pass filters with varying cutoff frequencies

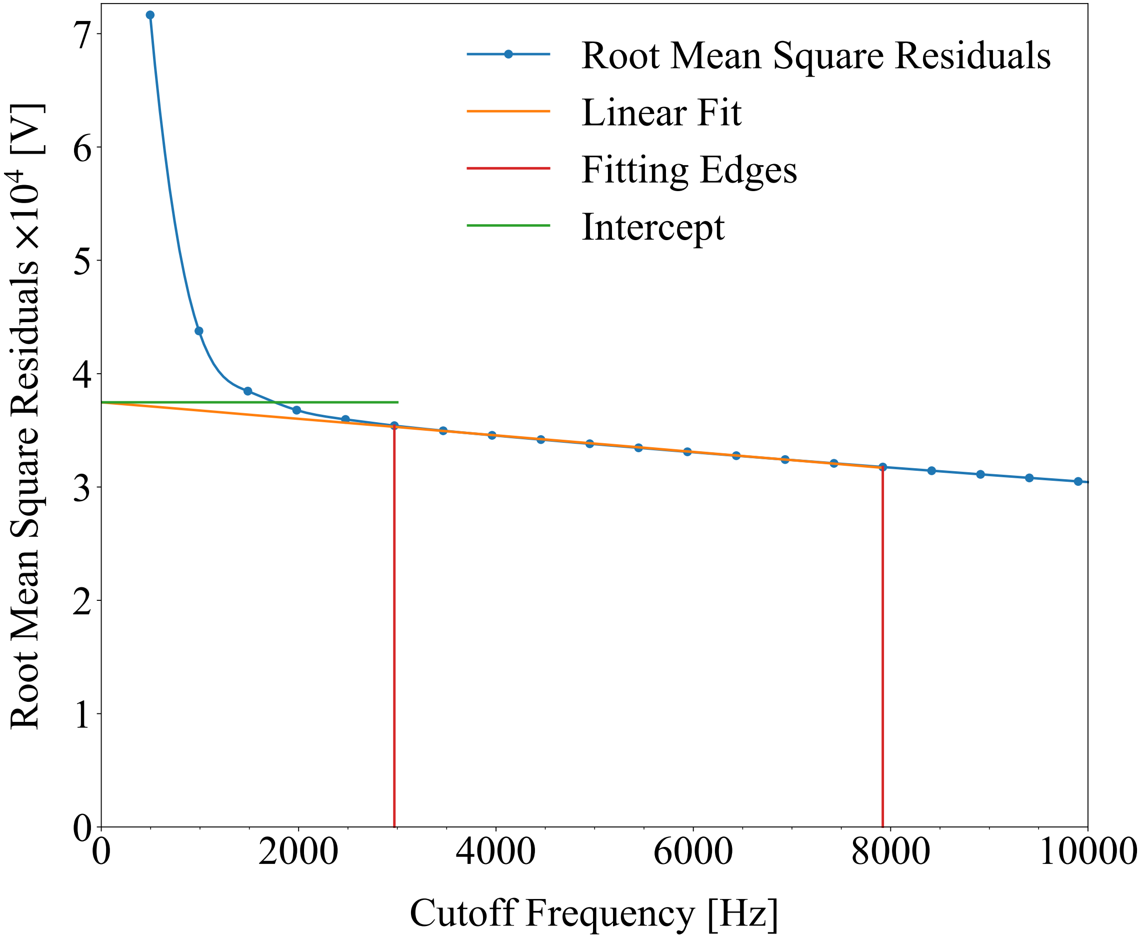
Filter the voltage trace and calculate the root mean square residual of the filtered signal relative to the original signal

Linear fit to residuals to select optimum



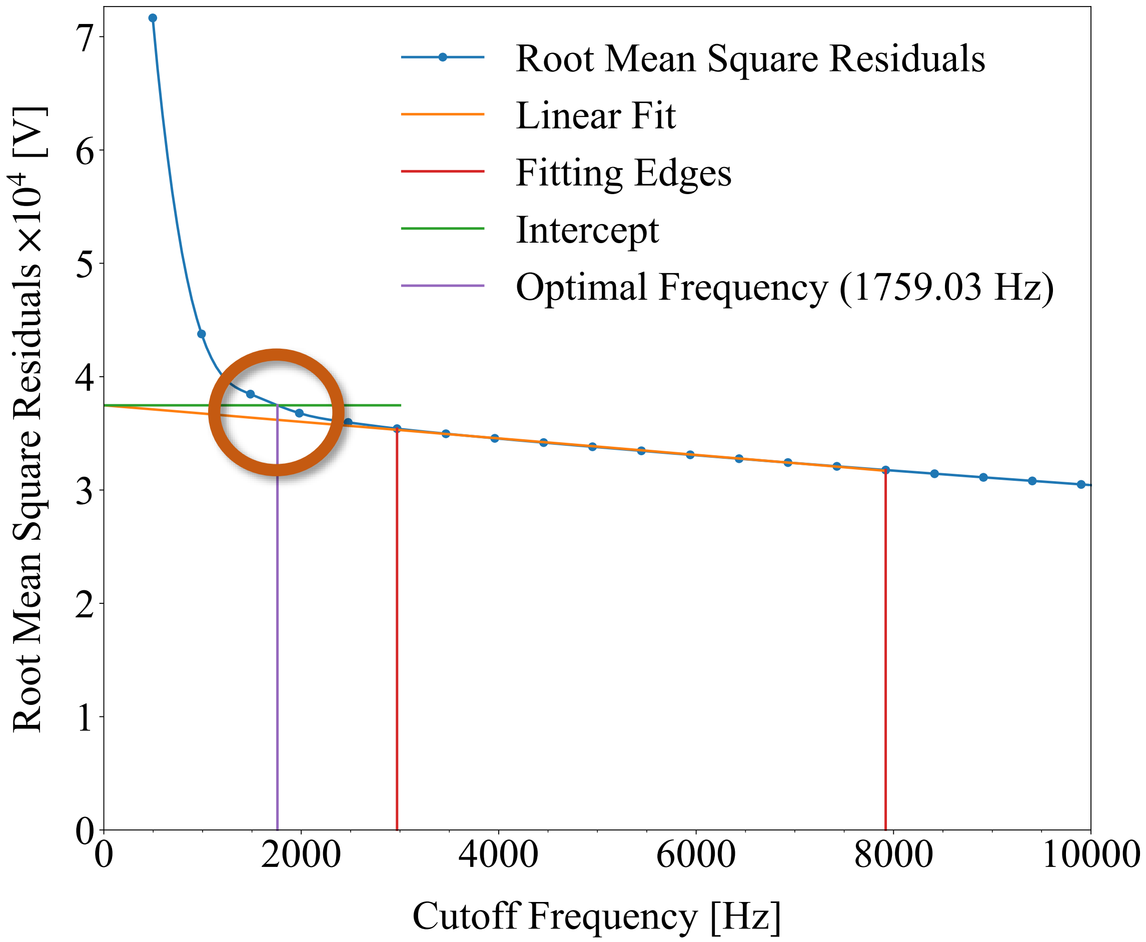
Duarte (2014) URL: https://goo.gl/GoCGfq
Yu et al. (1999) DOI: 10.1123/jab.15.3.318

Linear fit to residuals to select optimum



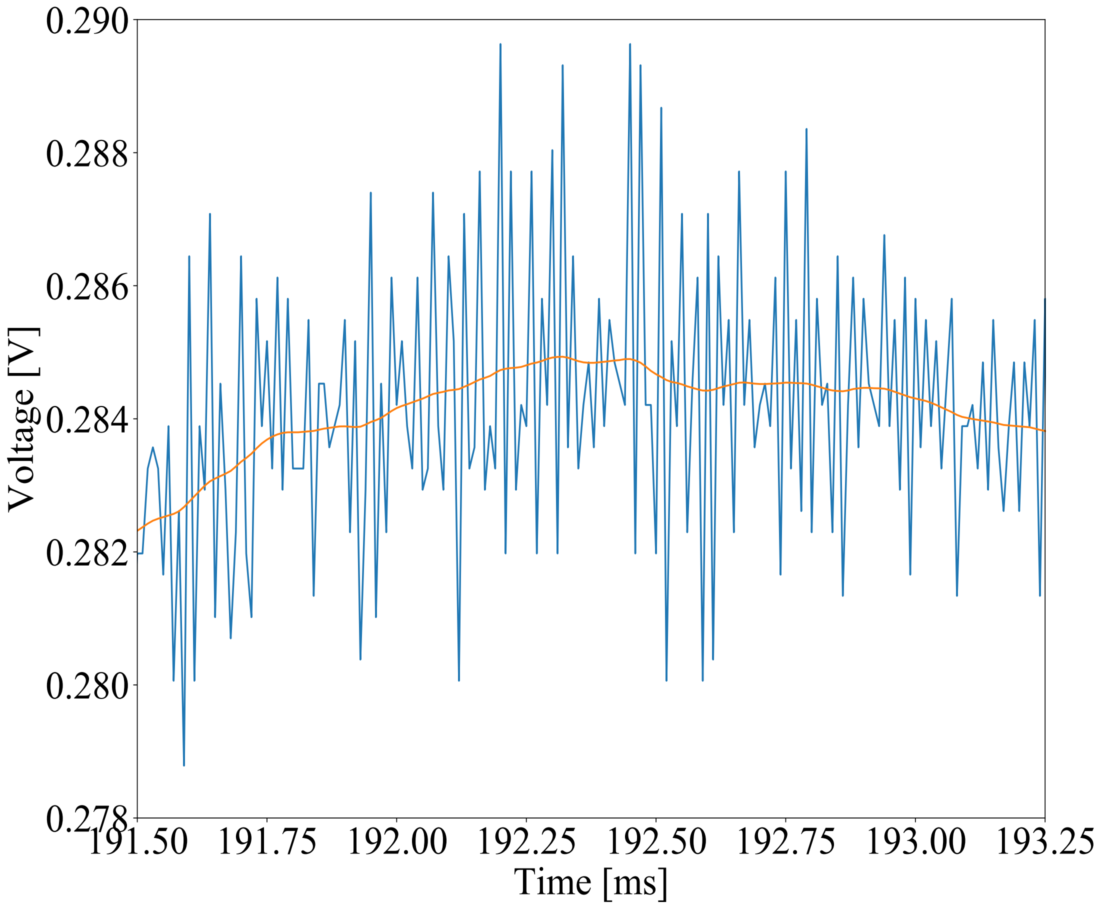
Duarte (2014) URL: https://goo.gl/GoCGfq
Yu et al. (1999) DOI: 10.1123/jab.15.3.318

Optimum where y-intercept crosses residuals

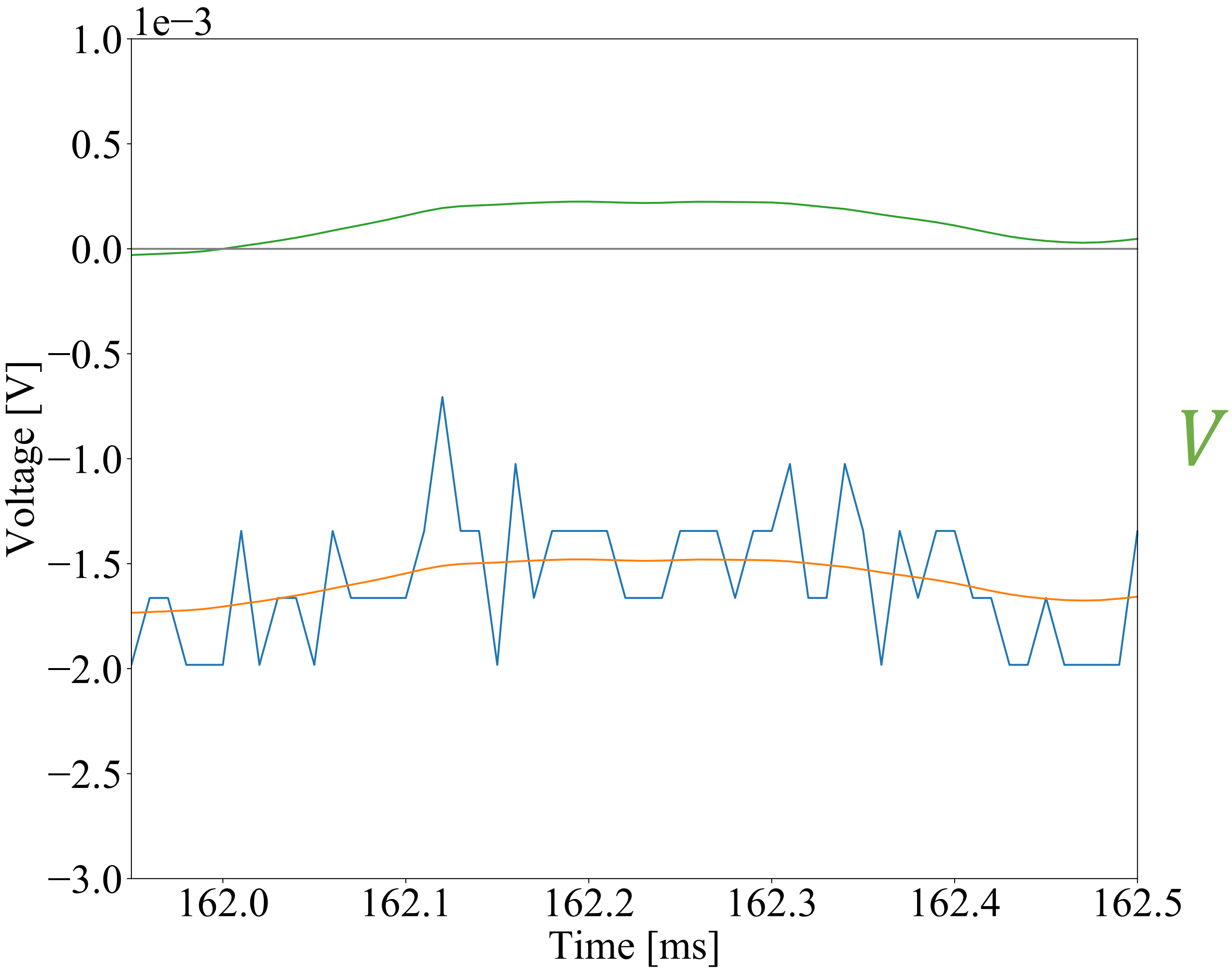


Duarte (2014) URL: https://goo.gl/GoCGfq
Yu et al. (1999) DOI: 10.1123/jab.15.3.318

Filtering the Voltage Trace

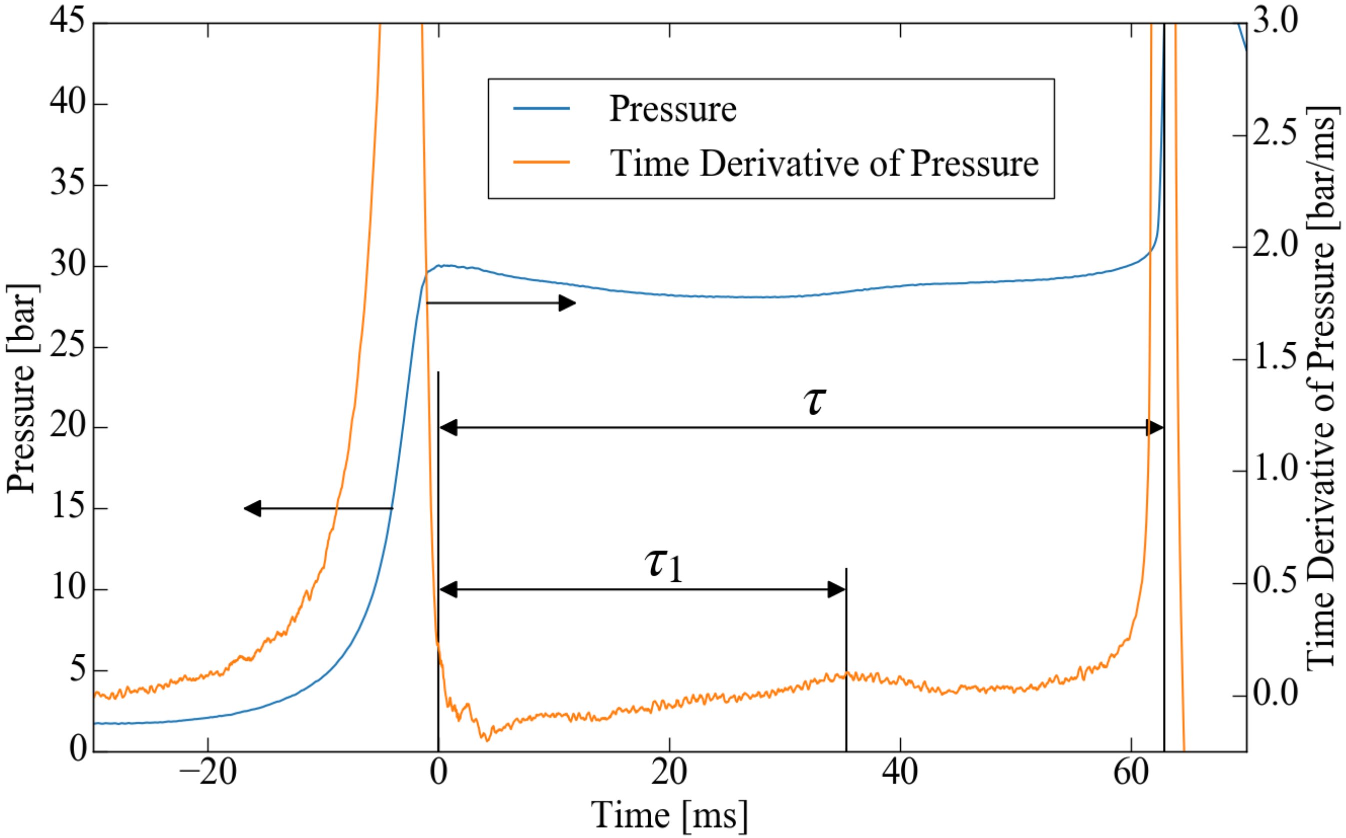


Correcting the Offset



$$V = \overline{V} - \overline{V}(0)$$

Computing Ignition Delay



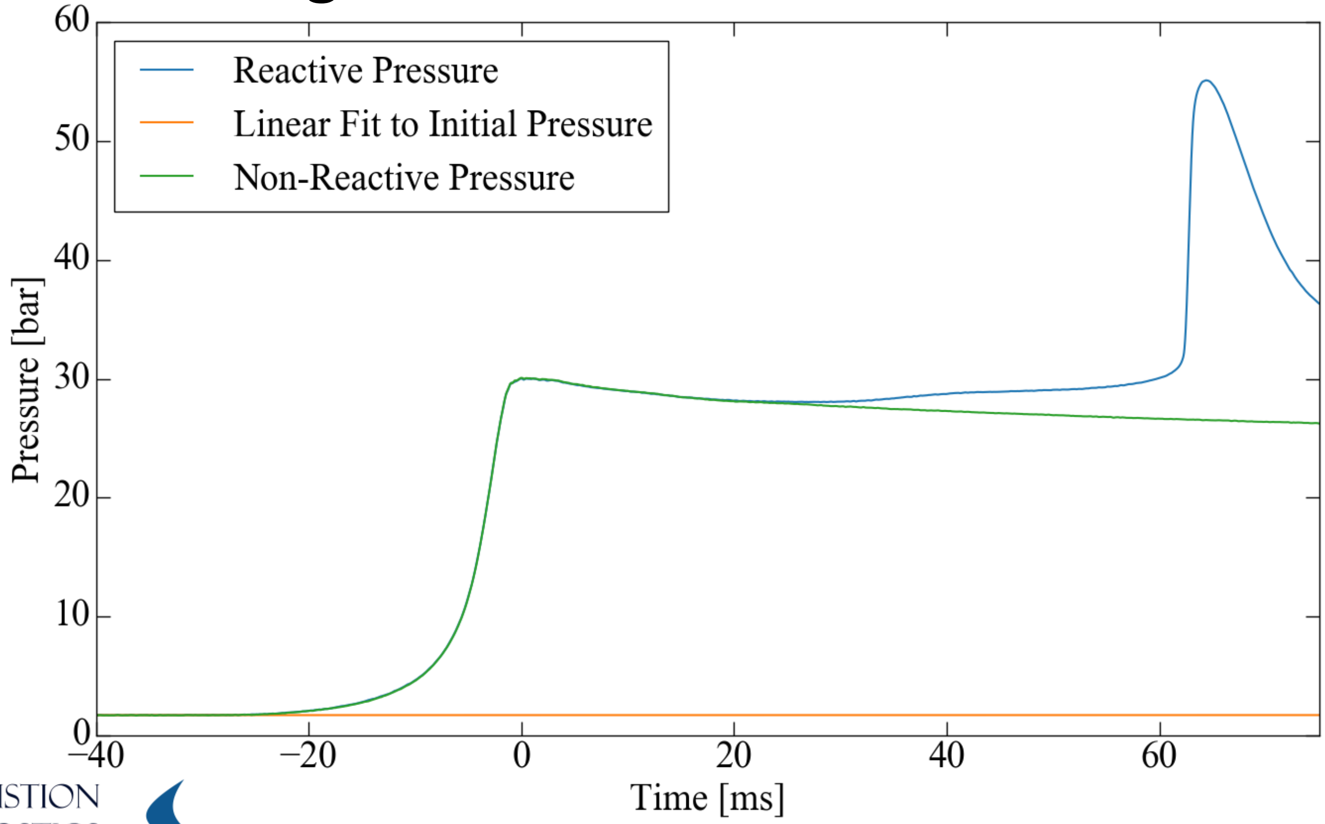
$$P = V * F + P_0$$

$$\tau = \max\left(\frac{dP}{dt}\right)$$

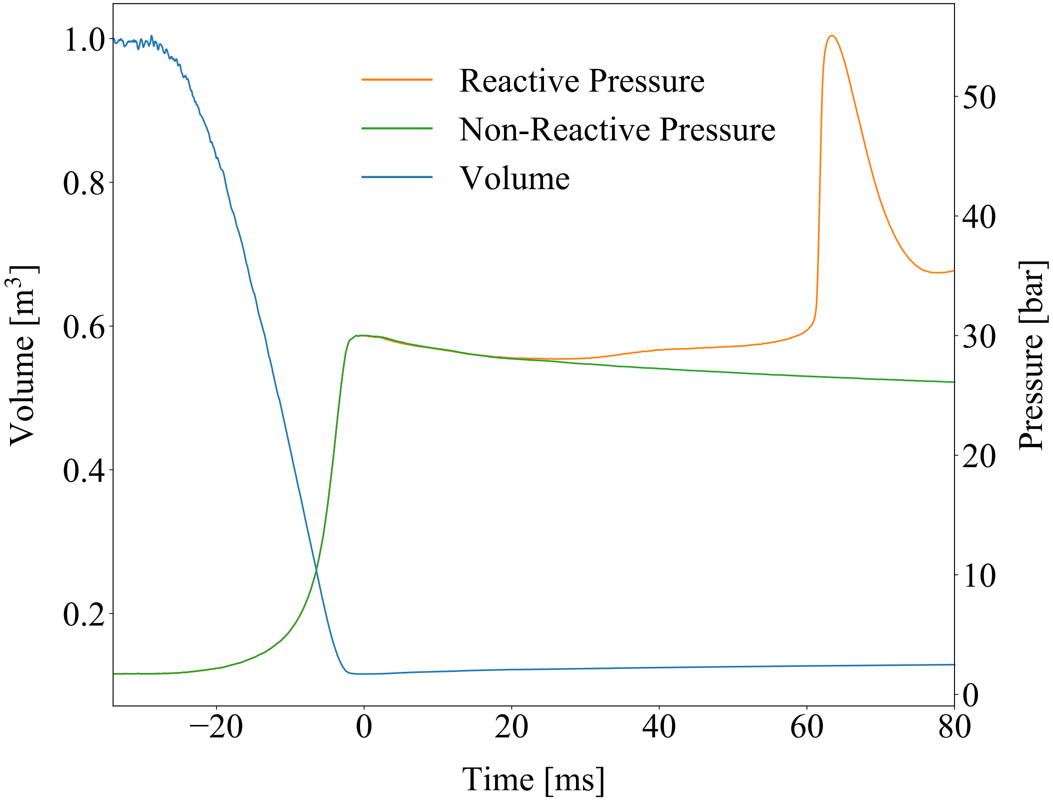
$\frac{dP}{dt}$ → Second order forward difference

Modeling facility effects

- Replace oxygen with nitrogen and run the experiment again



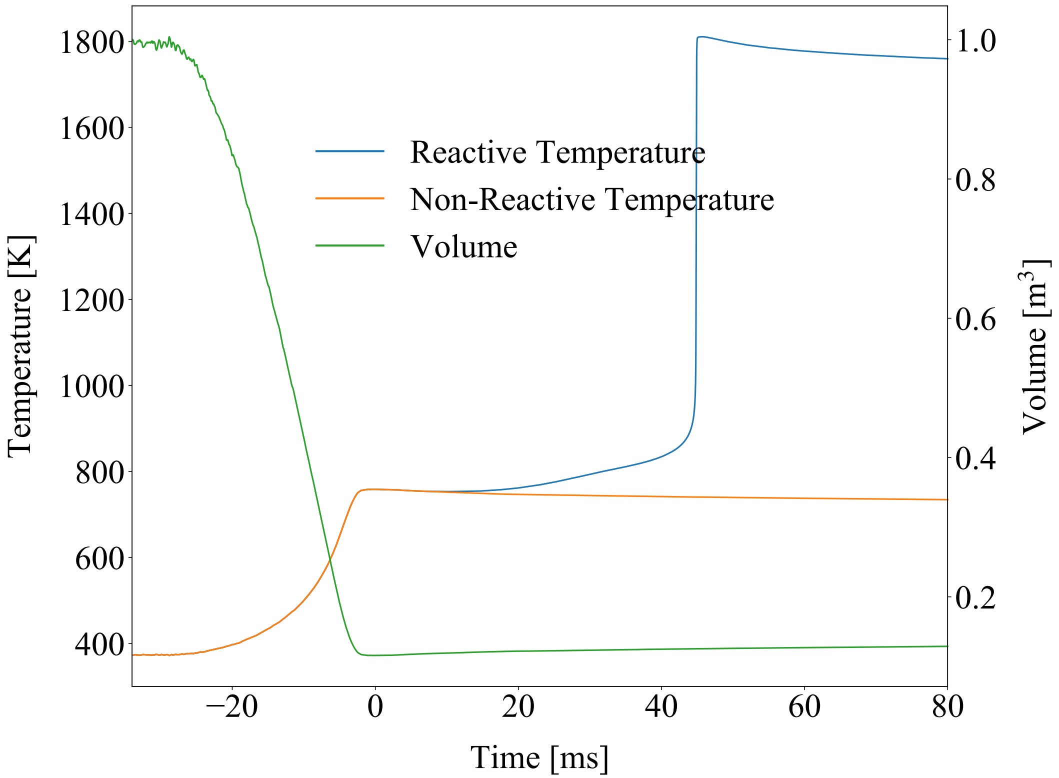
Modeling Facility Effects



Experimental Pressures

- Need the volume of the reactor as a function of time (not measured)
- Reaction chamber modeled as isentropic compression followed by isentropic expansion
- Volume trace calculated from pressure trace

Modeling Facility Effects



Simulated Temperature

- The temperature at the end of compression is found by applying the compression/expansion process to the law of conservation of energy

$$c_v \frac{dT}{dt} = -P\frac{dv}{dt} - \sum_k u_k \frac{dY_k}{dt}$$

- Non-reactive and reactive temperatures agree at the end of compression

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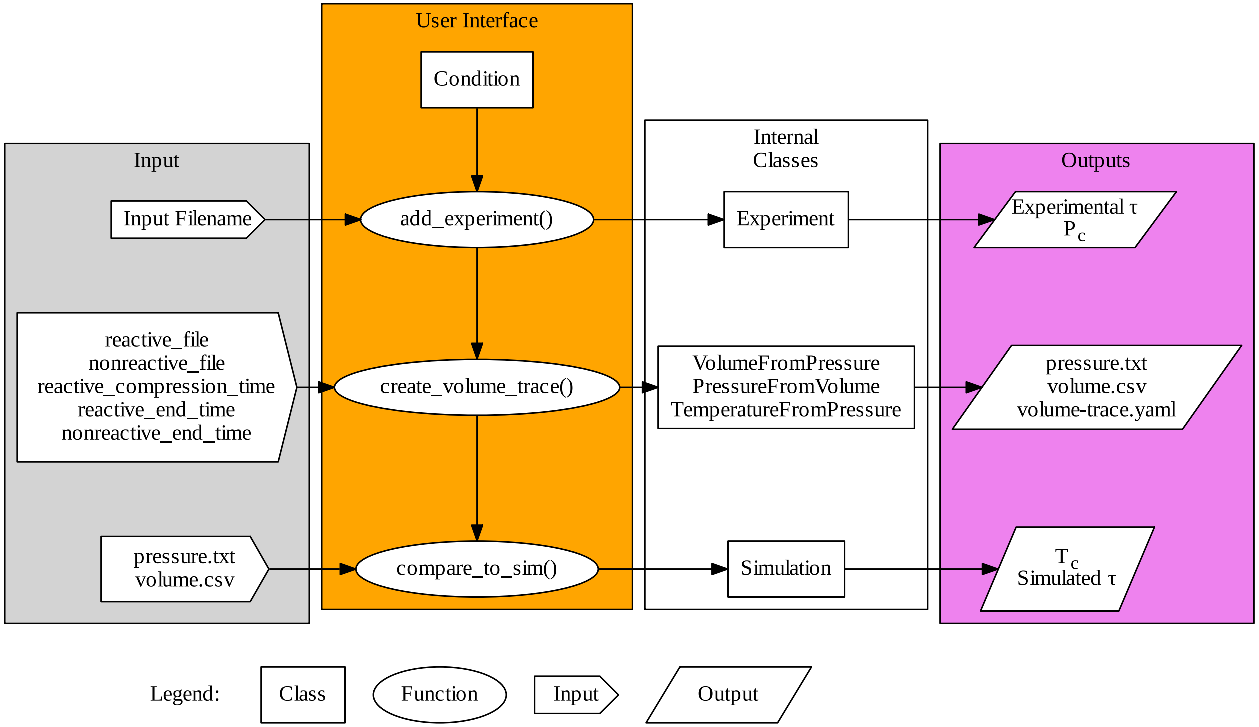
Outputs from UConnRCMPy

- We output the volume as a function of time for use in simulations
  - `volume.csv`
- We output the pressure as a function of time for comparison
  - `Tc_P0_T0_pressure.txt`
- We output the choices of important parameters relevant to reproducing the analysis
  - `volume_trace.yaml`
- We output the values of P_C, P_0, T_C, T_0, τ, and the optimal filter frequency for reporting

Modular Design

- Enables modifications for different file formats with consistent choices of filtering criteria, etc.



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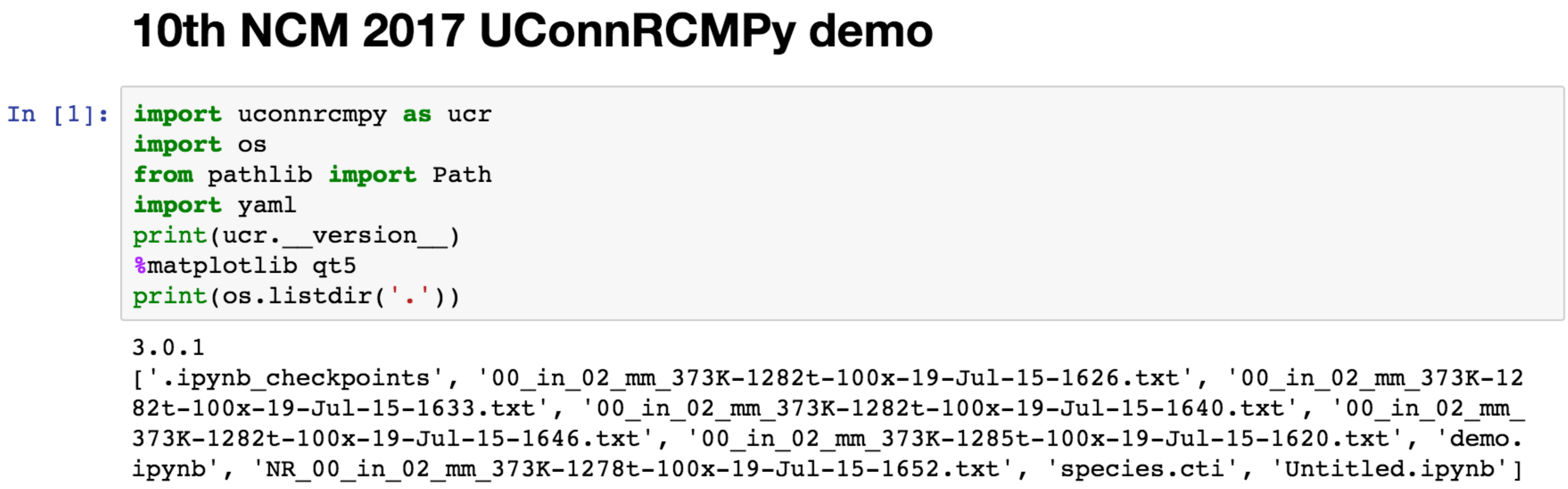
Scientific Python Software

- SciPy (https://github.com/scipy/scipy) for filter construction and convolution
- Cantera (https://github.com/Cantera/cantera) to calculate thermodynamic information about the reactor
- Matplotlib (https://github.com/matplotlib/matplotlib) for plots
- Documentation is available online (http://bryanwweber.github.io/UConnRCMPy/), generated by Sphinx

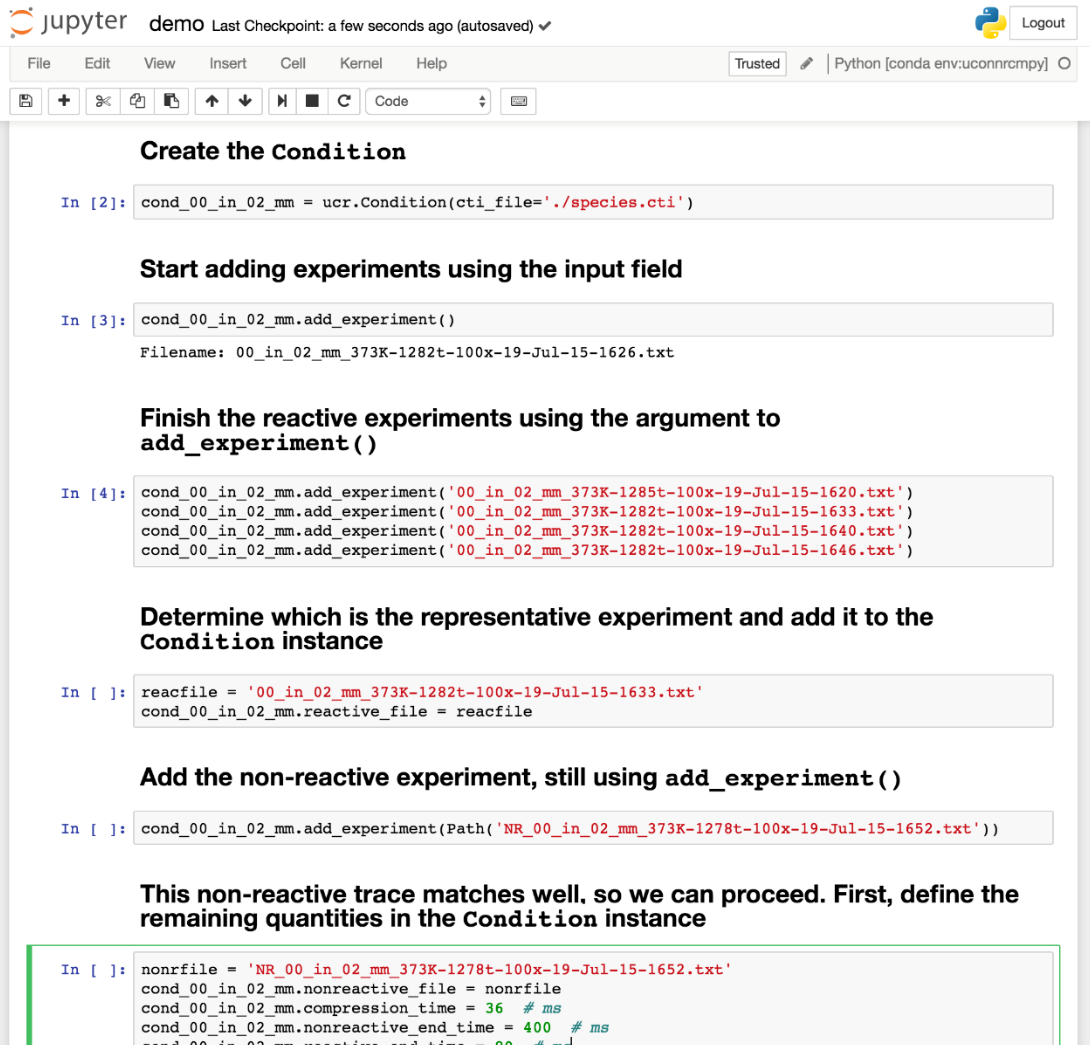
Demo



10th NCM 2017 UConnRCMPy demo

```
In [1]: import uconnrcmpy as ucr
        import os
        from pathlib import Path
        import yaml
        print(ucr.__version__)
        %matplotlib qt5
        print(os.listdir('.'))
```

```
3.0.1
['.ipynb_checkpoints', '00_in_02_mm_373K-1282t-100x-19-Jul-15-1626.txt', '00_in_02_mm_373K-12
82t-100x-19-Jul-15-1633.txt', '00_in_02_mm_373K-1282t-100x-19-Jul-15-1640.txt', '00_in_02_mm_
373K-1282t-100x-19-Jul-15-1646.txt', '00_in_02_mm_373K-1285t-100x-19-Jul-15-1620.txt', 'demo.
ipynb', 'NR_00_in_02_mm_373K-1278t-100x-19-Jul-15-1652.txt', 'species.cti', 'Untitled.ipynb']
```


jupyter
demo Last Checkpoint: a few seconds ago (autosaved)
Logout
File
Edit
View
Insert
Cell
Kernel
Help
Trusted
Python [conda env:uconnrcmpy]
Code

Create the `Condition`

```
In [2]: cond_00_in_02_mm = ucr.Condition(cti_file='./species.cti')
```

Start adding experiments using the input field

```
In [3]: cond_00_in_02_mm.add_experiment()

        Filename: 00_in_02_mm_373K-1282t-100x-19-Jul-15-1626.txt
```

Finish the reactive experiments using the argument to `add_experiment()`

```
In [4]: cond_00_in_02_mm.add_experiment('00_in_02_mm_373K-1285t-100x-19-Jul-15-1620.txt')
        cond_00_in_02_mm.add_experiment('00_in_02_mm_373K-1282t-100x-19-Jul-15-1633.txt')
        cond_00_in_02_mm.add_experiment('00_in_02_mm_373K-1282t-100x-19-Jul-15-1640.txt')
        cond_00_in_02_mm.add_experiment('00_in_02_mm_373K-1282t-100x-19-Jul-15-1646.txt')
```

Determine which is the representative experiment and add it to the `Condition` instance

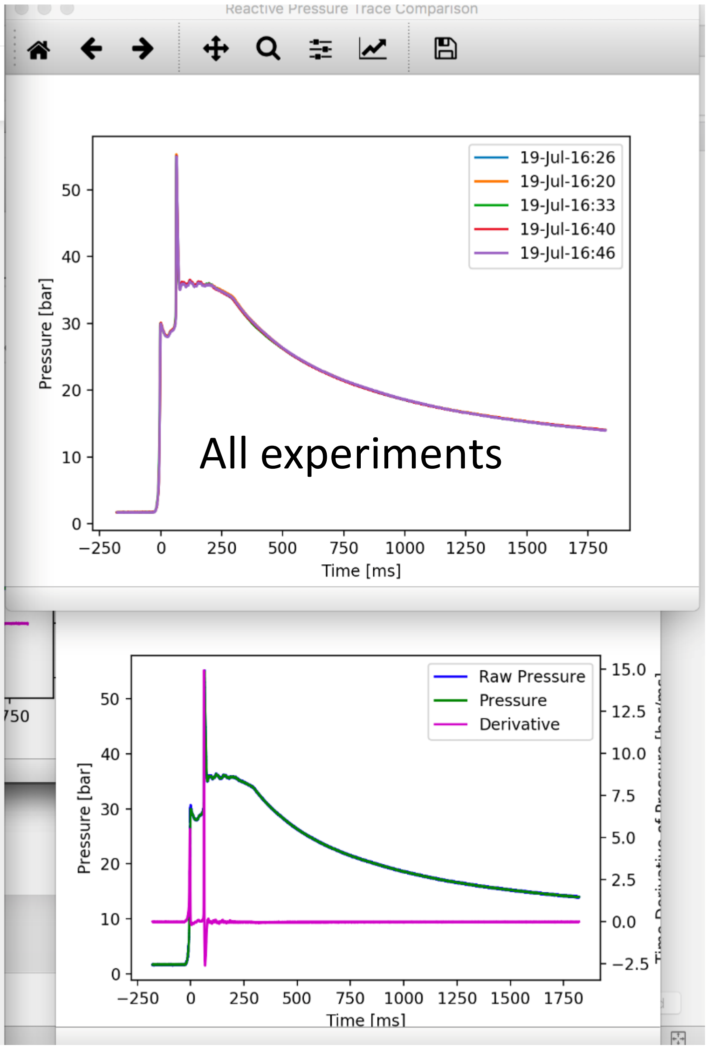
```
In [ ]: reacfile = '00_in_02_mm_373K-1282t-100x-19-Jul-15-1633.txt'
        cond_00_in_02_mm.reactive_file = reacfile
```

Add the non-reactive experiment, still using `add_experiment()`

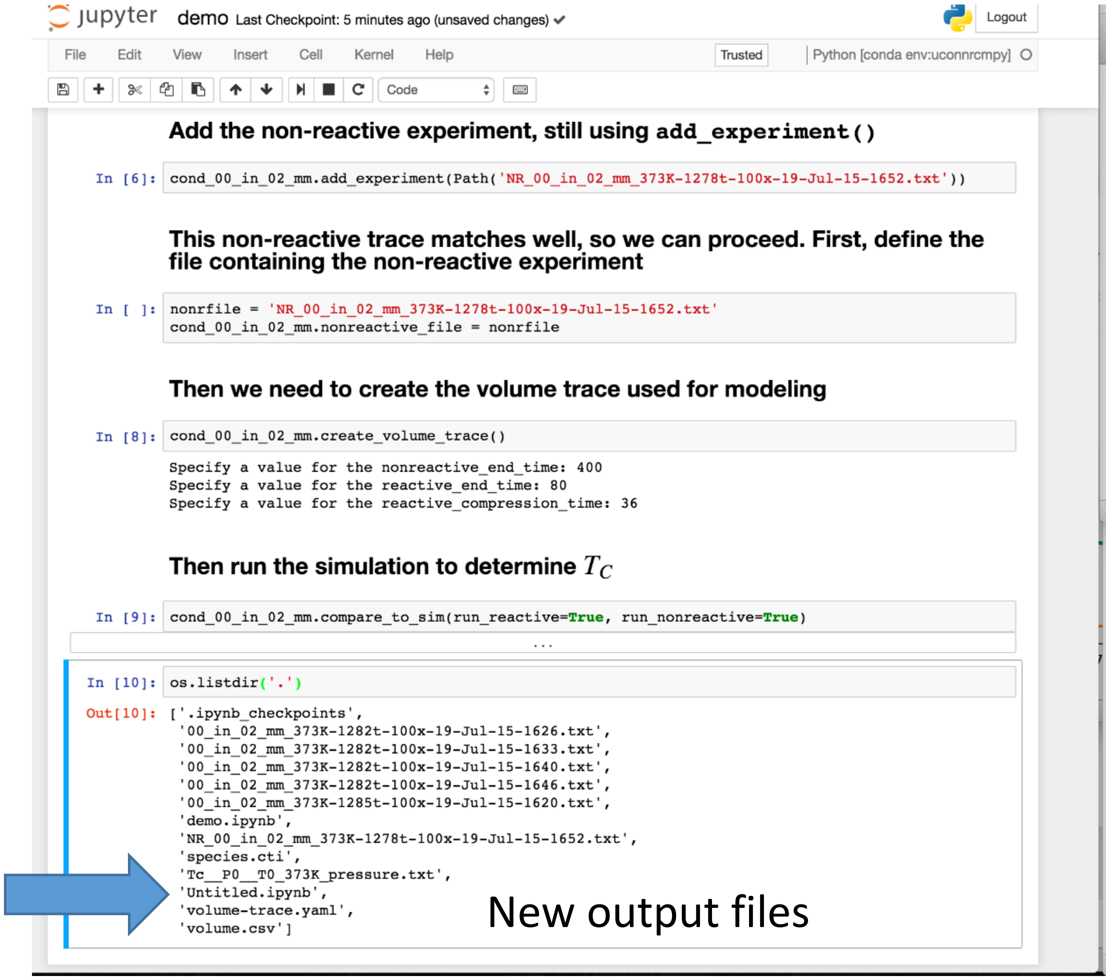
```
In [ ]: cond_00_in_02_mm.add_experiment(Path('NR_00_in_02_mm_373K-1278t-100x-19-Jul-15-1652.txt'))
```

This non-reactive trace matches well, so we can proceed. First, define the remaining quantities in the `Condition` instance

```
In [ ]: nonrfile = 'NR_00_in_02_mm_373K-1278t-100x-19-Jul-15-1652.txt'
        cond_00_in_02_mm.nonreactive_file = nonrfile
        cond_00_in_02_mm.compression_time = 36  # ms
        cond_00_in_02_mm.nonreactive_end_time = 400  # ms
```



Single Experiment


jupyter demo Last Checkpoint: 5 minutes ago (unsaved changes)
Logout
File Edit View Insert Cell Kernel Help
Trusted
Python [conda env:uconnrcmpy]
Code

Add the non-reactive experiment, still using `add_experiment()`

```
In [6]: cond_00_in_02_mm.add_experiment(Path('NR_00_in_02_mm_373K-1278t-100x-19-Jul-15-1652.txt'))
```

This non-reactive trace matches well, so we can proceed. First, define the file containing the non-reactive experiment

```
In [ ]: nonrfile = 'NR_00_in_02_mm_373K-1278t-100x-19-Jul-15-1652.txt'
        cond_00_in_02_mm.nonreactive_file = nonrfile
```

Then we need to create the volume trace used for modeling

```
In [8]: cond_00_in_02_mm.create_volume_trace()

        Specify a value for the nonreactive_end_time: 400
        Specify a value for the reactive_end_time: 80
        Specify a value for the reactive_compression_time: 36
```

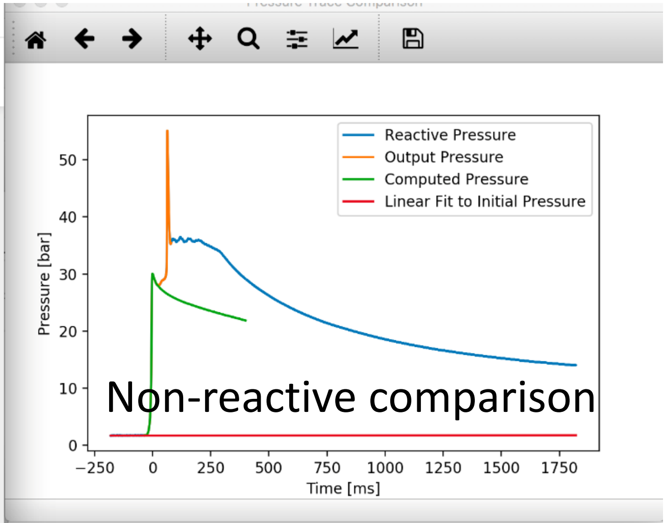
Then run the simulation to determine T_C

```
In [9]: cond_00_in_02_mm.compare_to_sim(run_reactive=True, run_nonreactive=True)
        ...
```

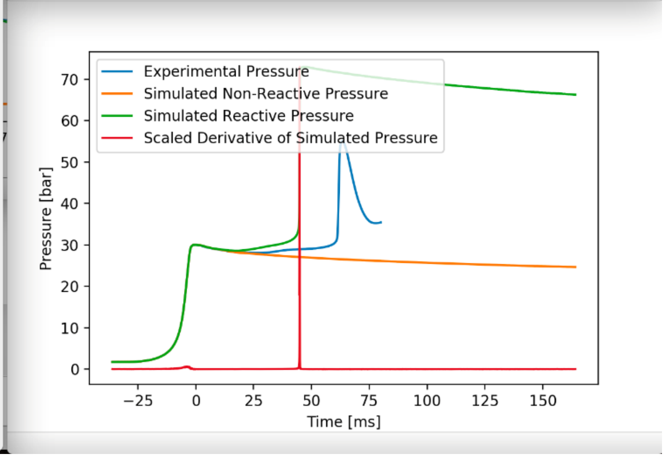
```
In [10]: os.listdir('.')

Out[10]: ['.ipynb_checkpoints',
          '00_in_02_mm_373K-1282t-100x-19-Jul-15-1626.txt',
          '00_in_02_mm_373K-1282t-100x-19-Jul-15-1633.txt',
          '00_in_02_mm_373K-1282t-100x-19-Jul-15-1640.txt',
          '00_in_02_mm_373K-1282t-100x-19-Jul-15-1646.txt',
          '00_in_02_mm_373K-1285t-100x-19-Jul-15-1620.txt',
          'demo.ipynb',
          'NR_00_in_02_mm_373K-1278t-100x-19-Jul-15-1652.txt',
          'species.cti',
          'Tc__P0__T0_373K_pressure.txt',
          'Untitled.ipynb',
          'volume-trace.yaml',
          'volume.csv']
```

New output files



Non-reactive comparison



Full simulation

Installation

```
conda install -c bryanwweber uconnrcmpy

pip install uconnrcmpy
```

Future Work

- Improved detection of the EOC
- Improved detection of two-stage ignition
- (More) unit testing!
- See https://github.com/bryanwweber/UConnRCMPy/issues

Acknowledgements

This work was funded by the National Science Foundation under Grant No. CBET-1402231

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