UConnRCMPy: Python-based Data Analysis for Rapid Compression Machines

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Combustion drives the energy economy

- Combustion is expected to remain the dominant energy conversion mechanism for many years
- The combustion of fossil fuels has been implicated in a number of harmful effects on human health, the environment, and the economy
- Two solutions have been proposed:
  - Better engines
  - Better fuels

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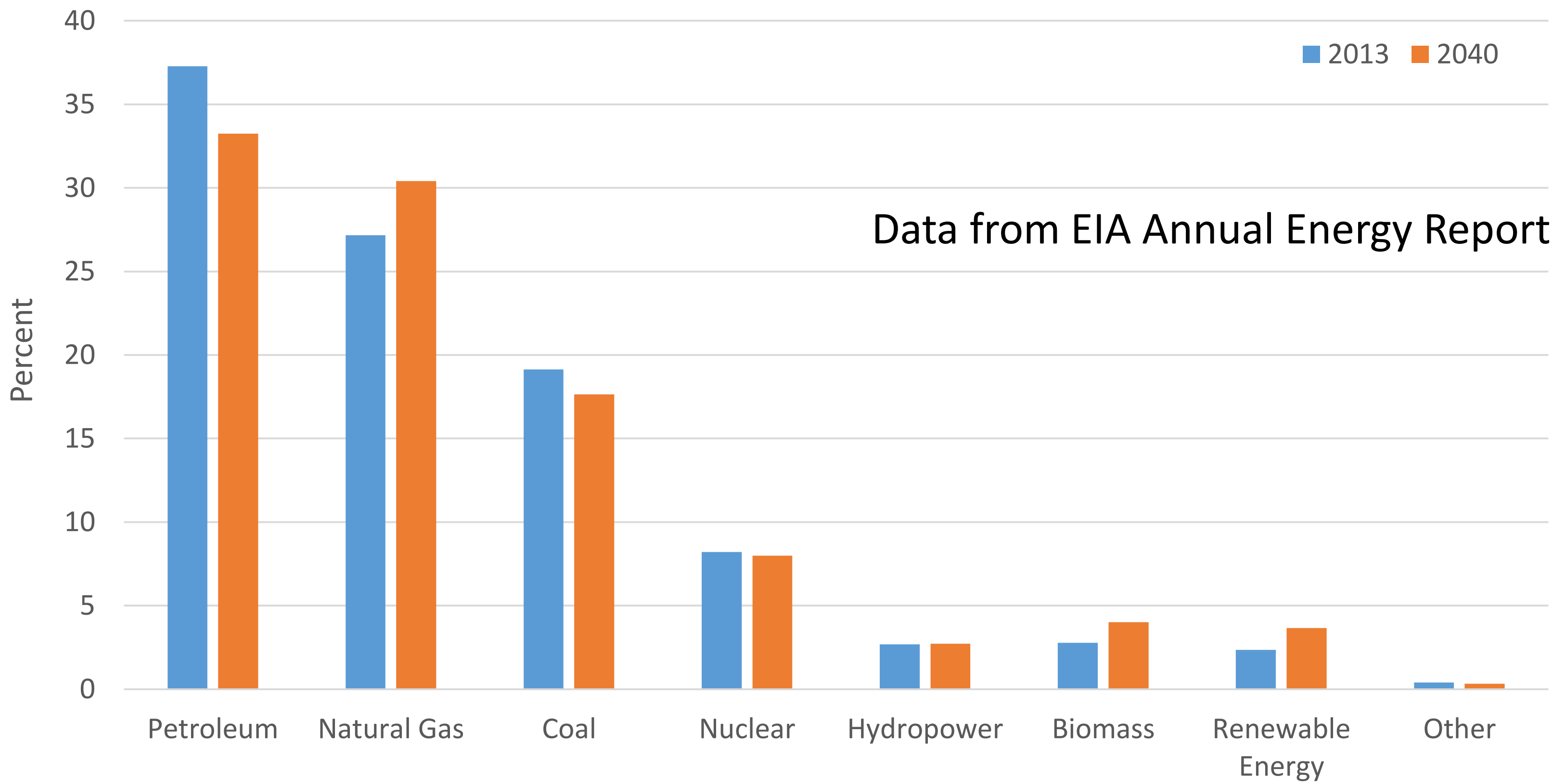
Combustion drives the energy economy



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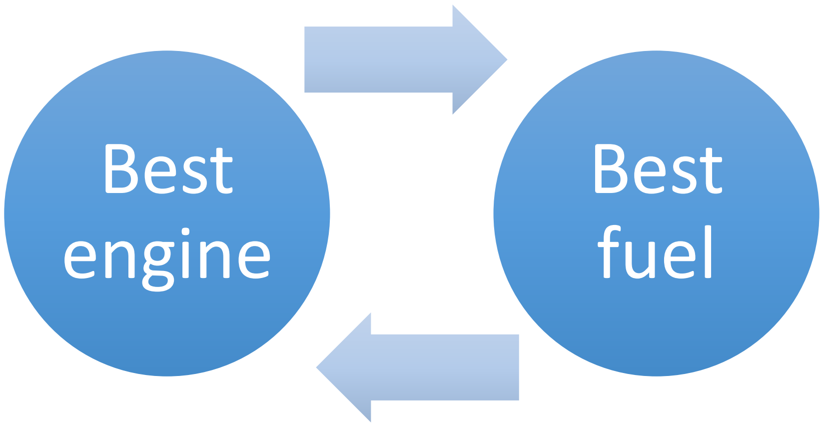
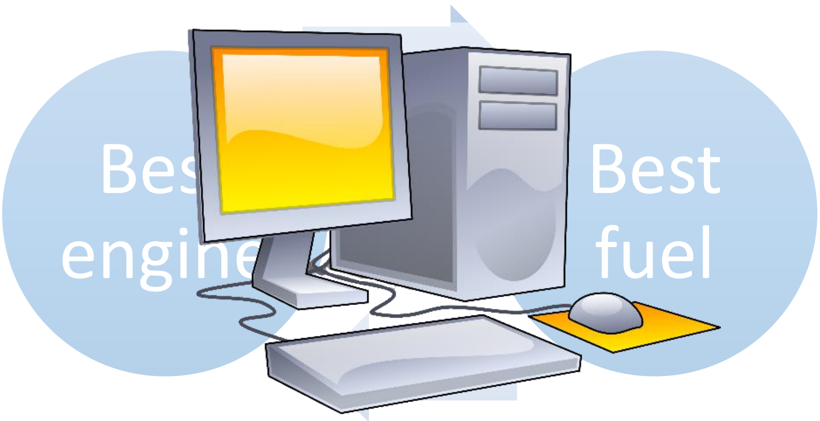
We need both solutions to make substantial progress

- Selecting the best alternative fuel requires knowledge of the best engine design, which requires deciding which is the best fuel…
- Testing every fuel in every engine is too expensive and too time consuming



We need both solutions to make substantial progress

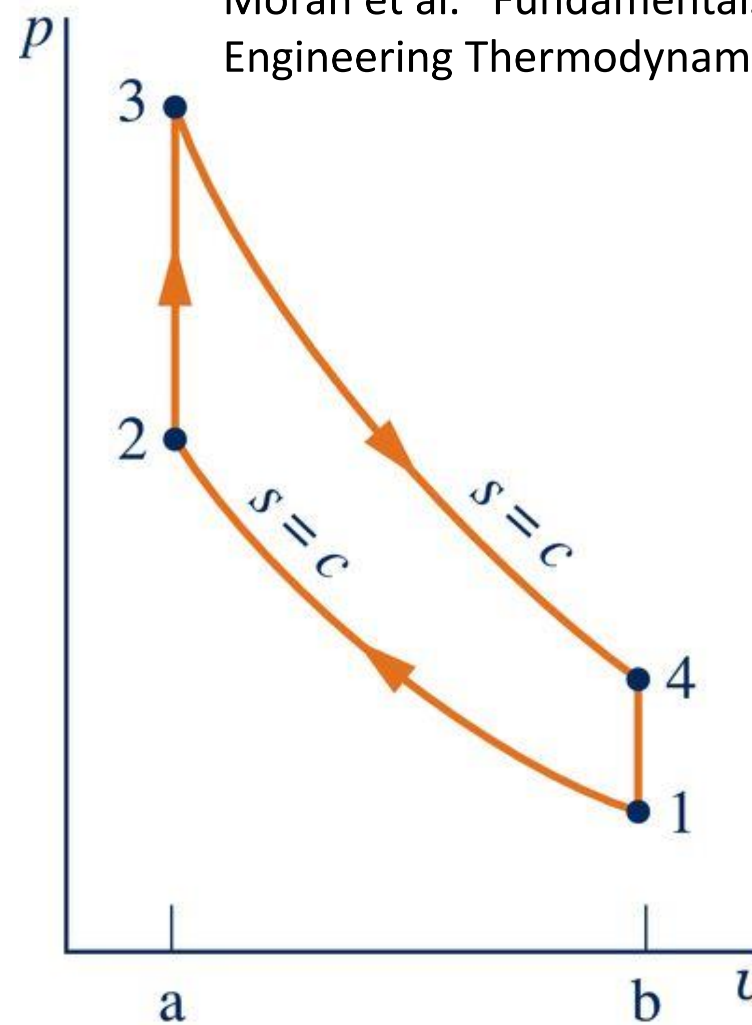
- Computer-aided design can be employed to design fuel-flexible, high-efficiency, low-emissions engines if the models we use are predictive



We want to do experiments that model a real engine

- Real engines operate at high pressure and low temperature
- Real engines are affected by:
  - Intake/Exhaust
  - Inhomogeneity
  - Fluid Mechanics
  - Power output

Moran et al. “Fundamentals of Engineering Thermodynamics” 8e



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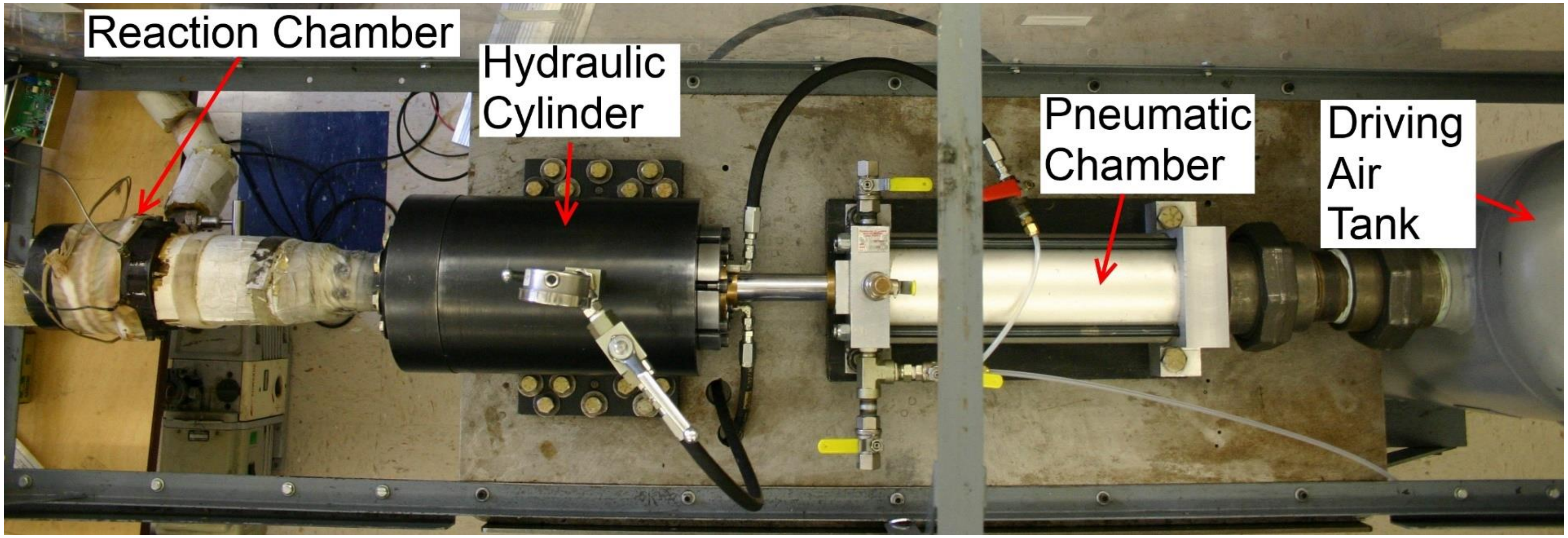
Rapid Compression Machine

- Experiments are conducted in a Rapid Compression Machine (RCM)
- High pressure and low temperature conditions
- Minimal effects of fluid mechanics and inhomogeneity



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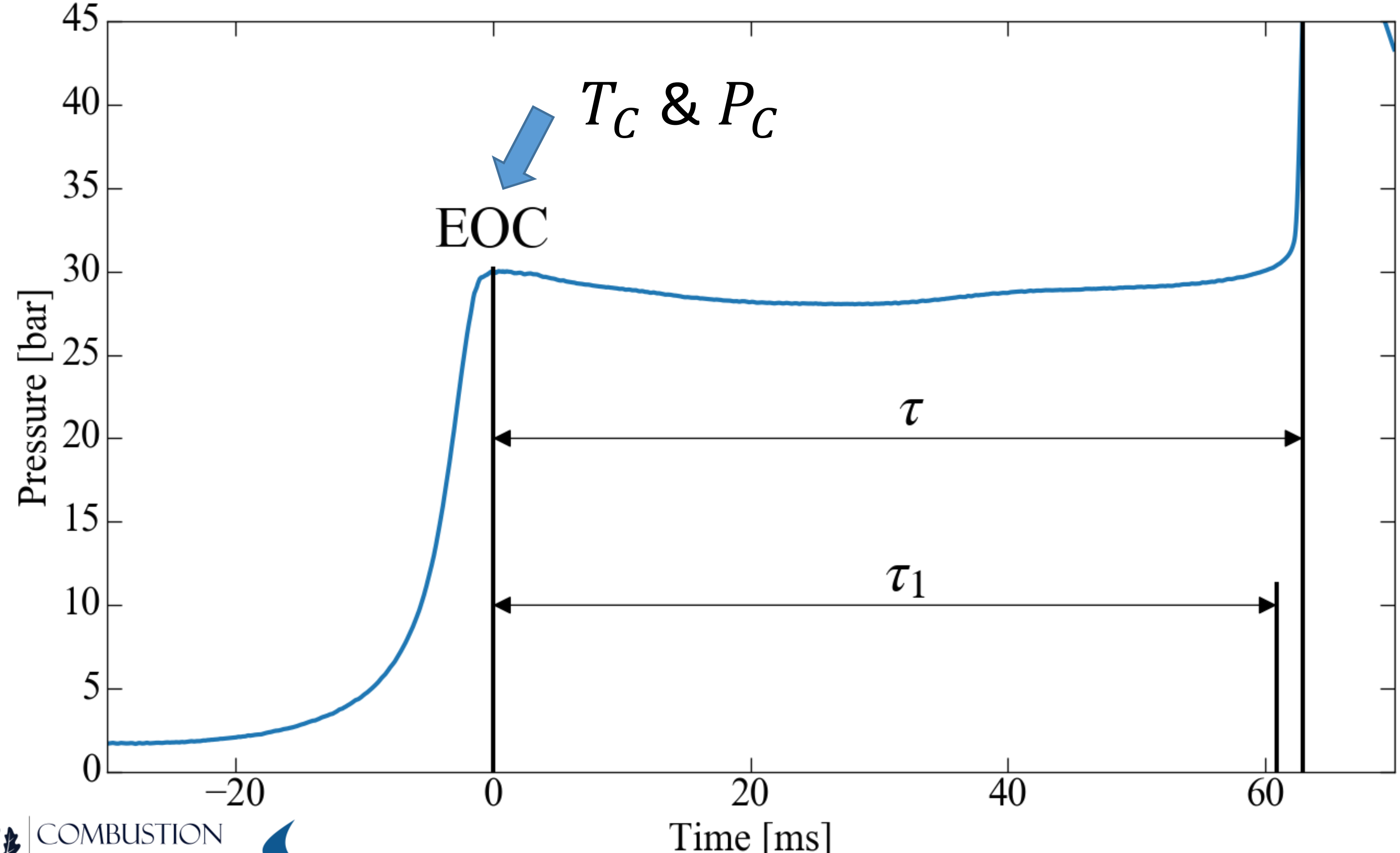
Rapid Compression Machine



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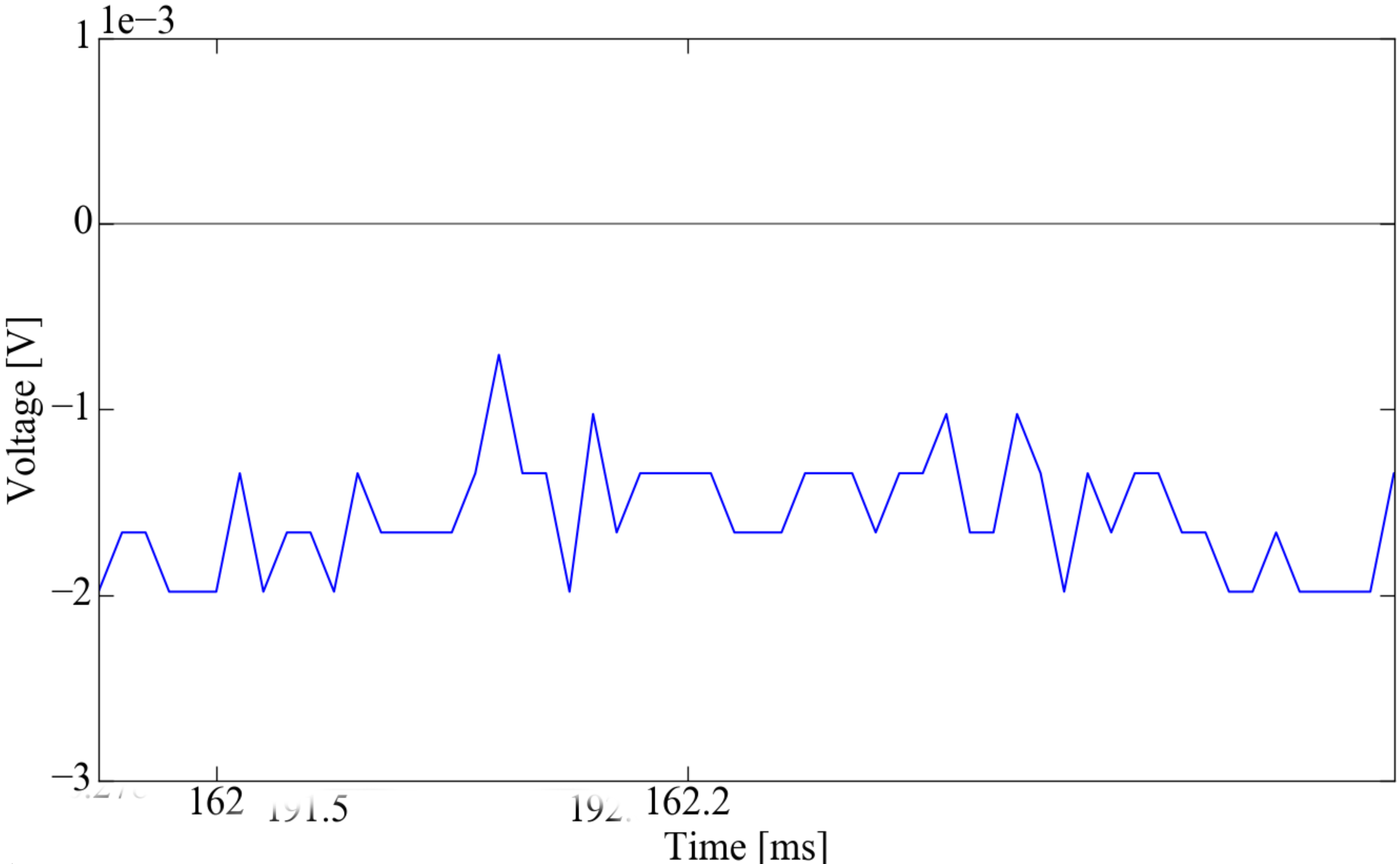
What do we measure?

- The reaction chamber pressure is the primary measurement in the RCM
- 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
- The voltage must be processed to compute the pressure, temperature, and ignition delay

What do we measure?



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~~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 data analysis procedure
- Reproducibility is important!

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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

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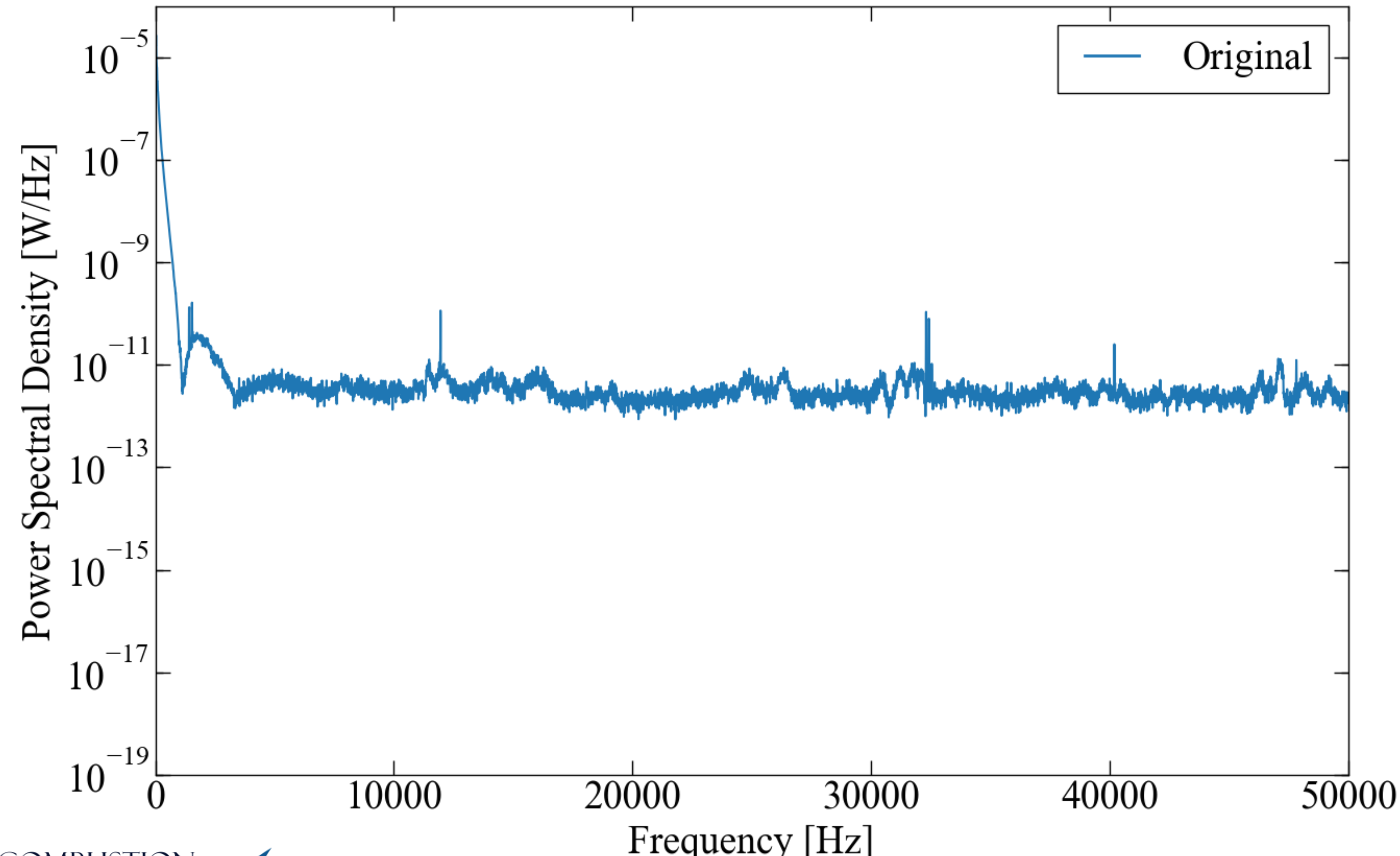
Features of UConnRCMPy

- Filtering and smoothing the raw voltage generated by the pressure transducer
- Converting the voltage trace into a pressure trace using settings recorded from the equipment
- Processing the pressure trace to determine parameters of interest in reporting the experiments, including the ignition delay and machine-specific effects on the experiment
- Conducting simulations utilizing the experimental information to calculate the temperature during the experiment

Filtering and Smoothing



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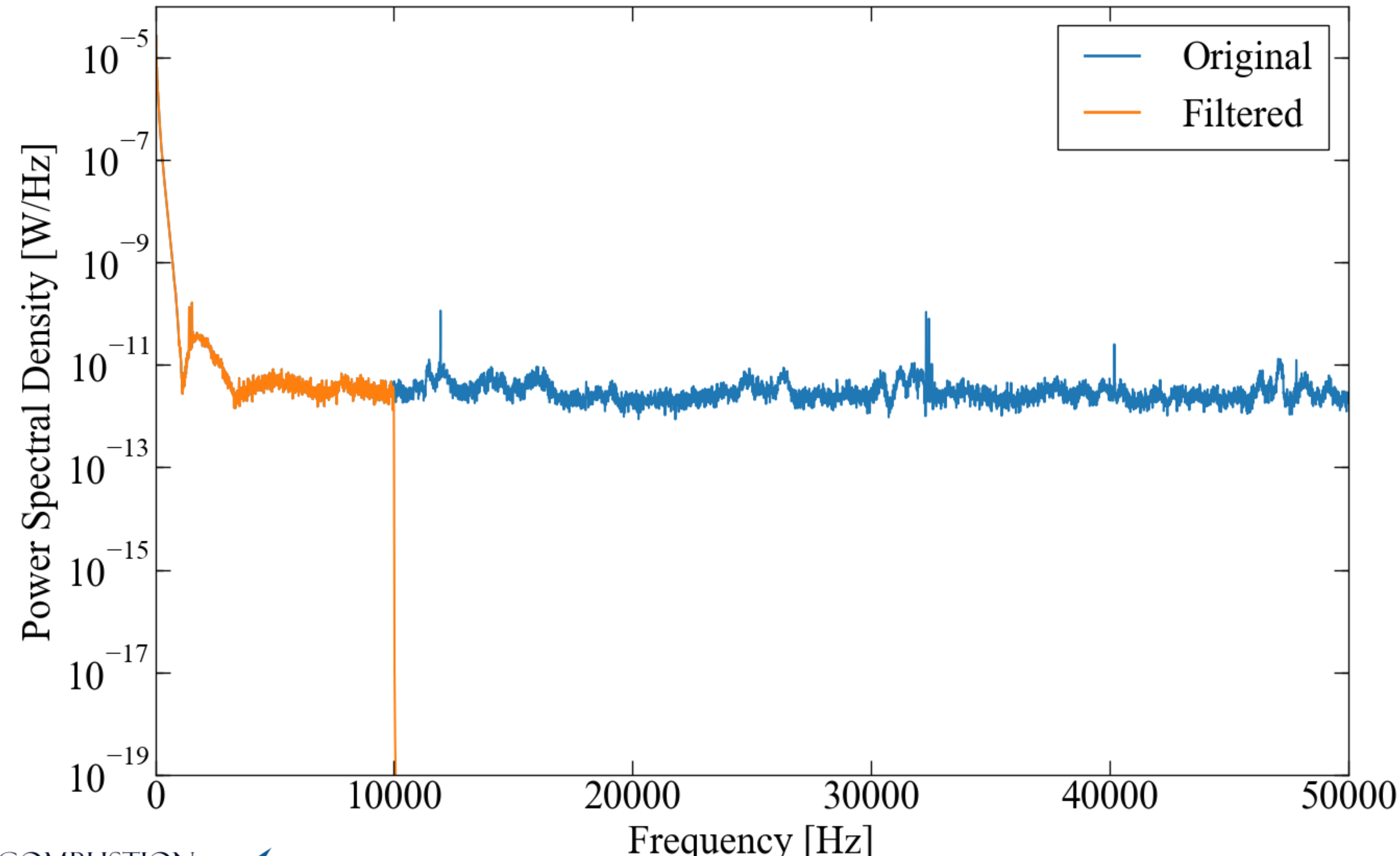
Filtering and Smoothing



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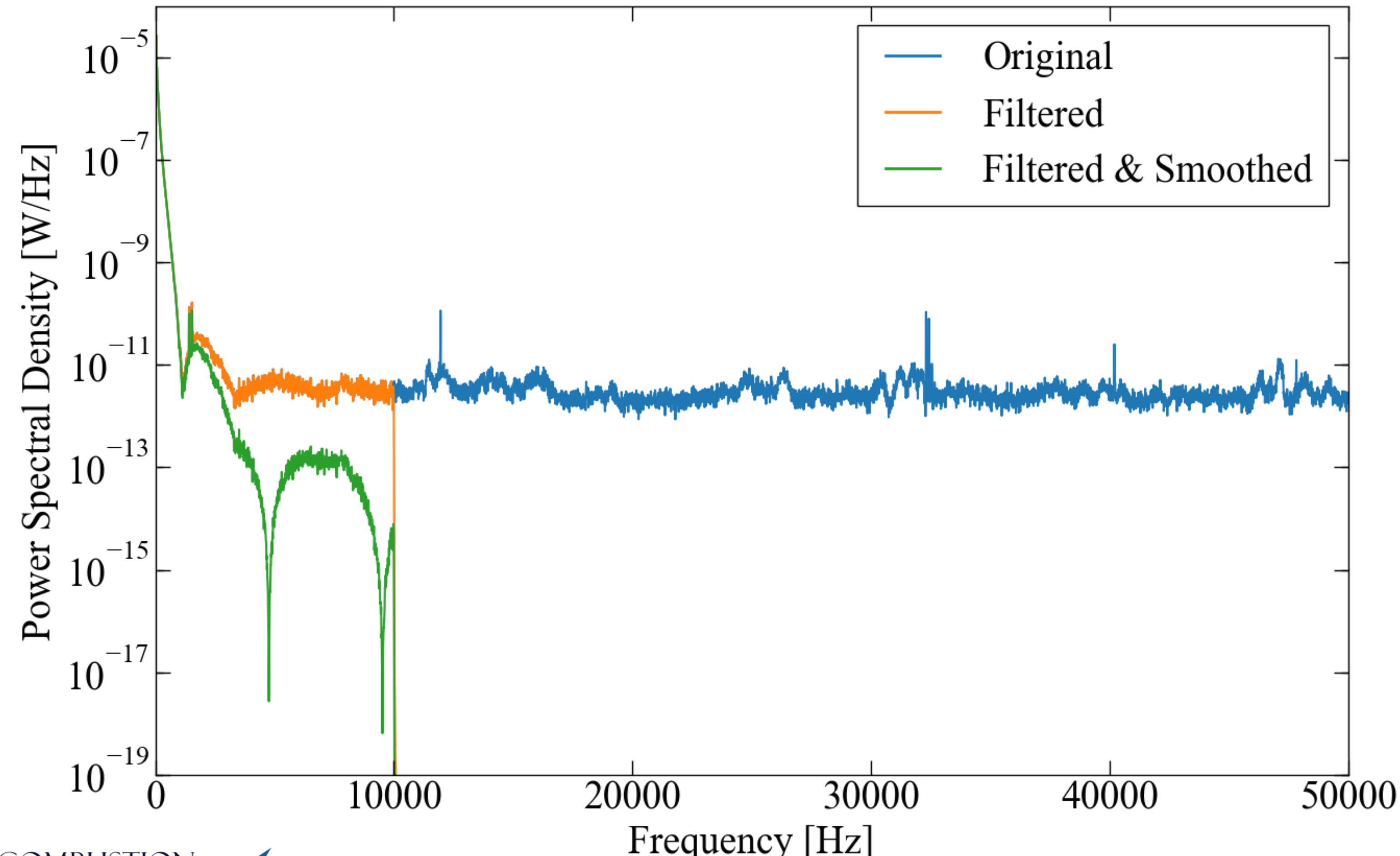
Filtering and Smoothing



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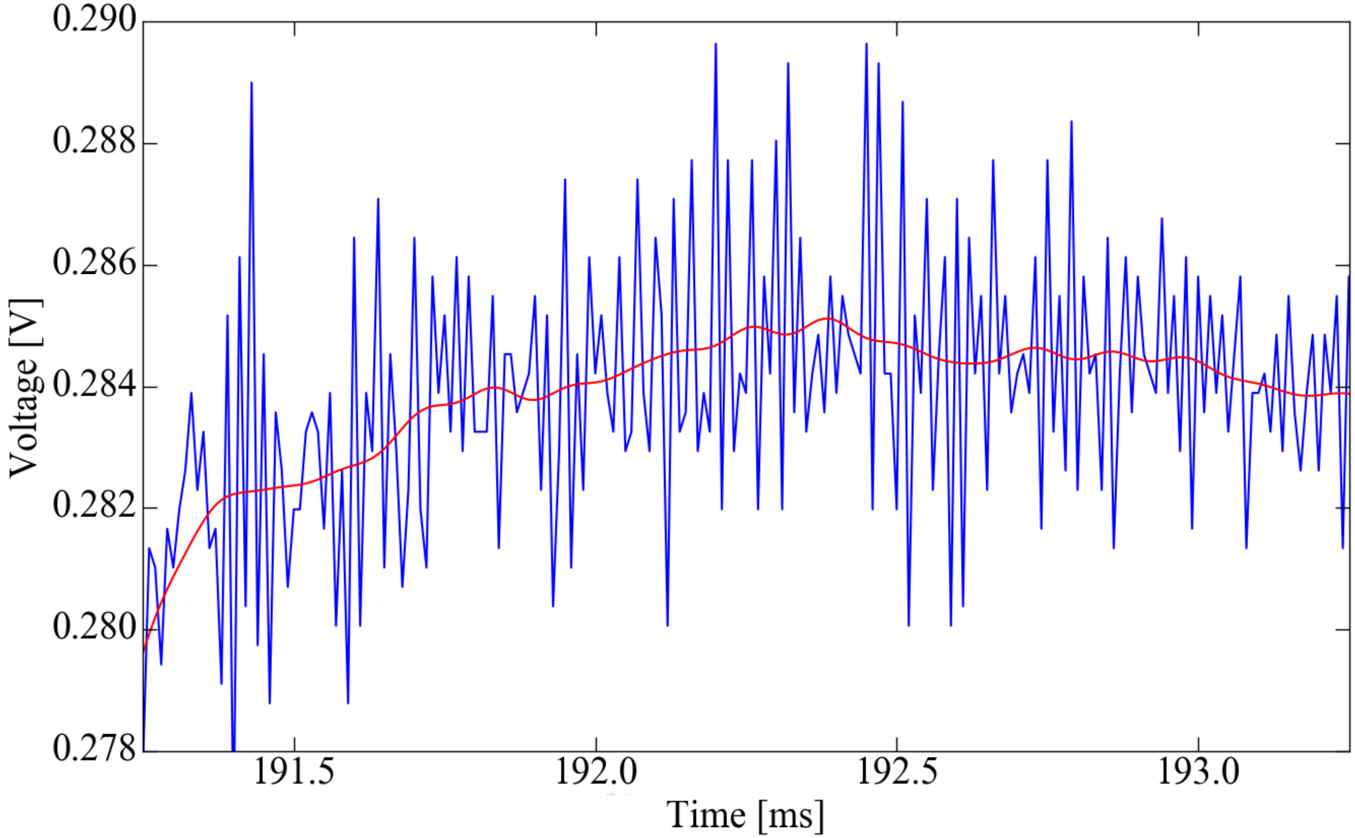
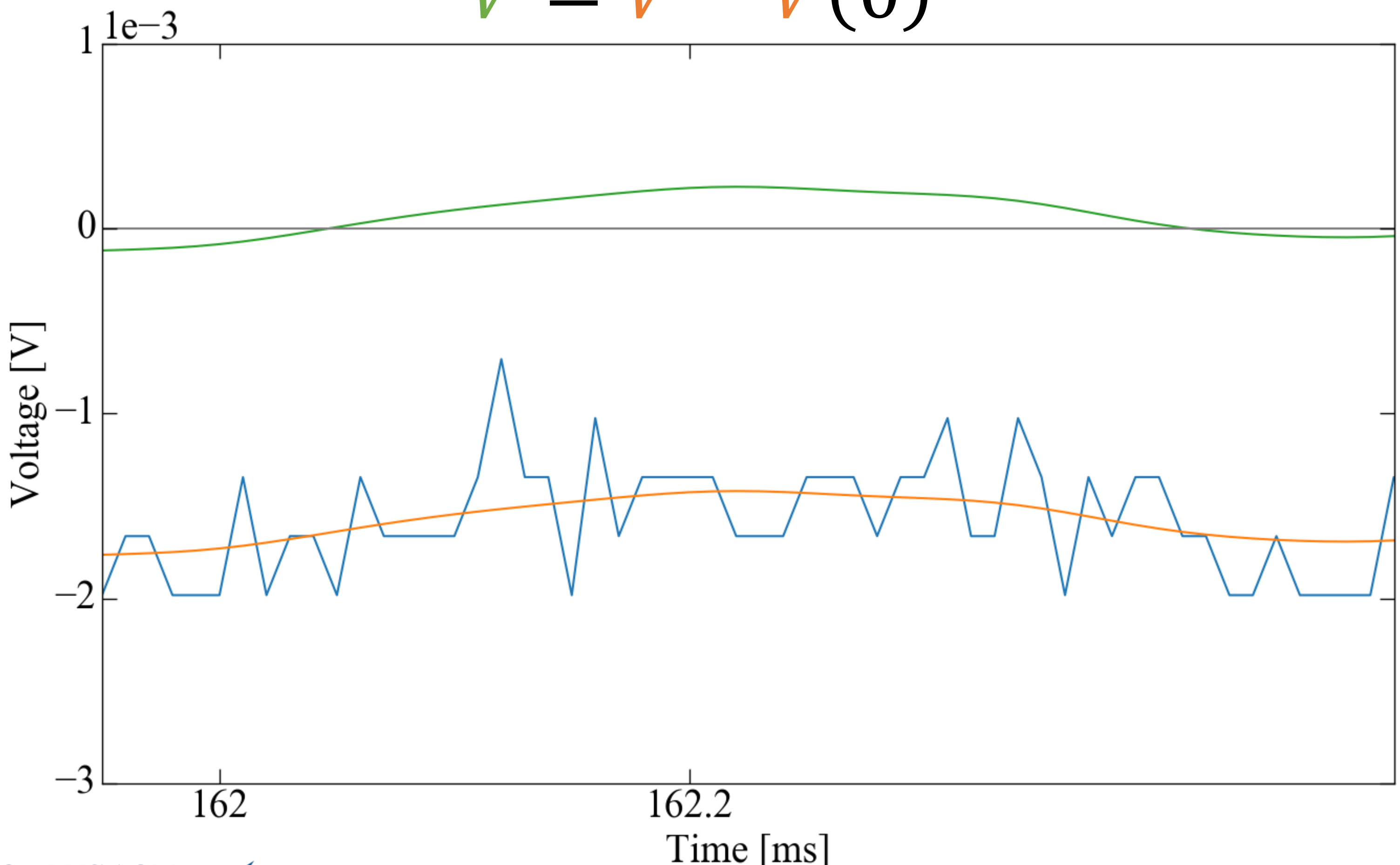
Filtering and Smoothing



Correcting the Offset

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



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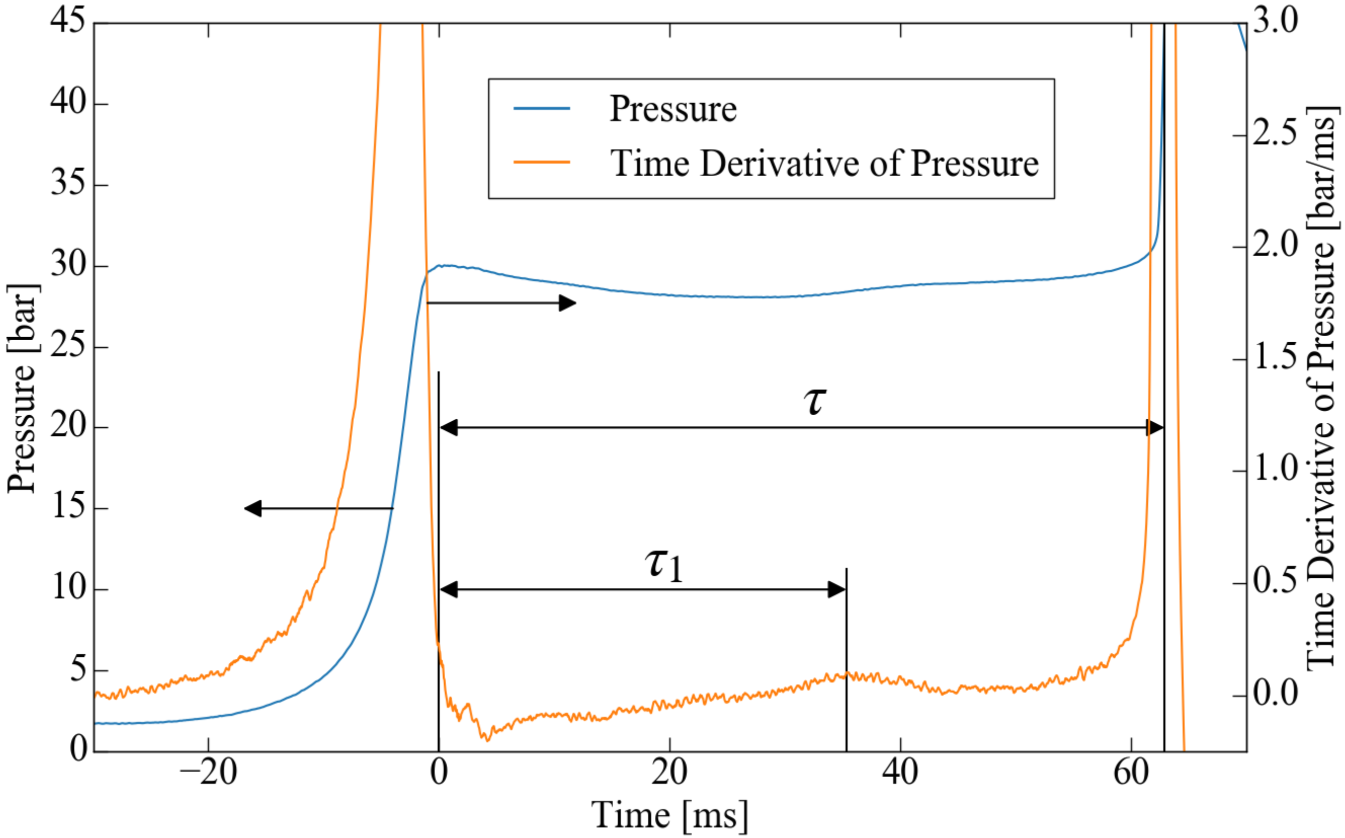
Computing Ignition Delay



$$P = V * F + P_0$$

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

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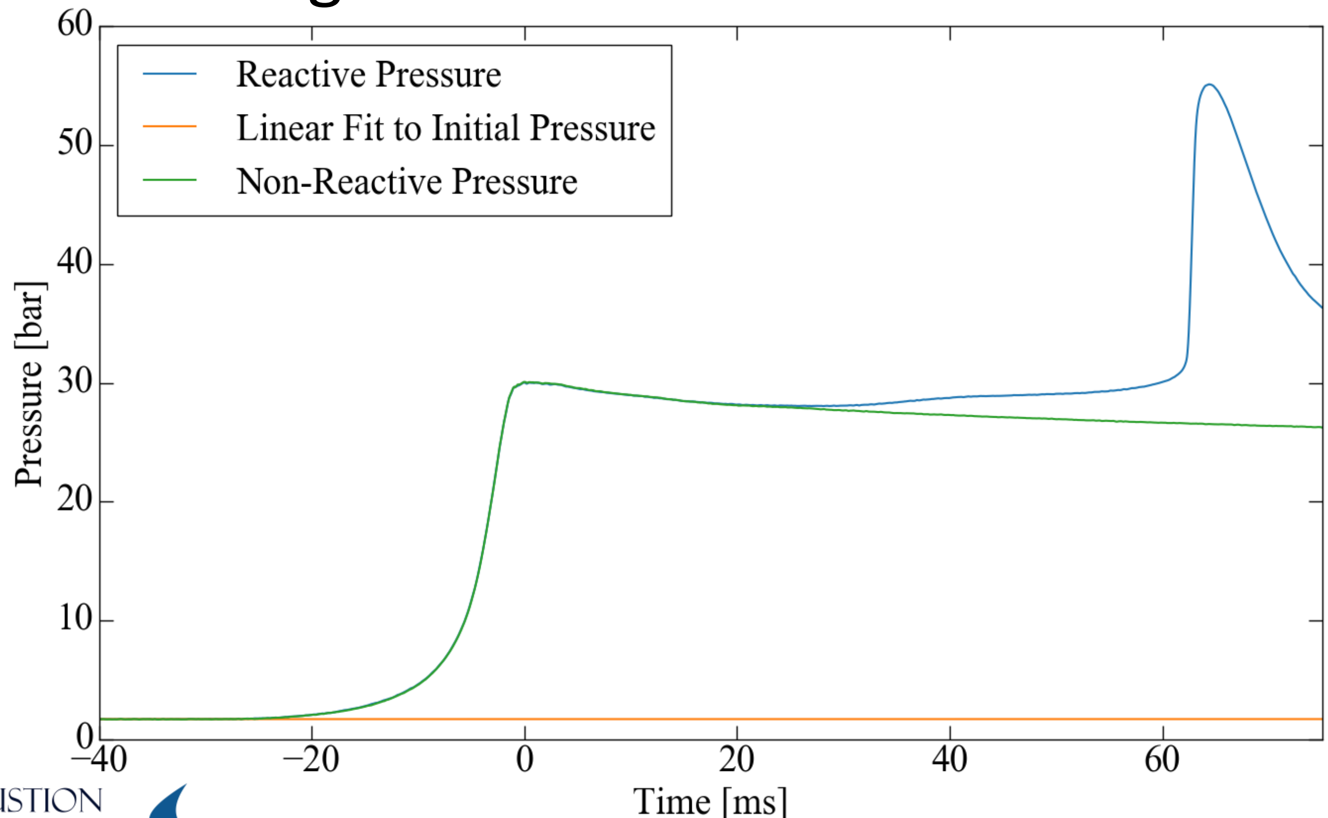
Modeling facility effects

- Replace oxygen with nitrogen and run the experiment again



Modeling Facility Effects

- The reaction chamber is modeled as undergoing adiabatic compression followed by adiabatic expansion, to reproduce the non-reactive pressure trace
- The temperature at the EOC is found by applying the compression/expansion process to the law of conservation of energy

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

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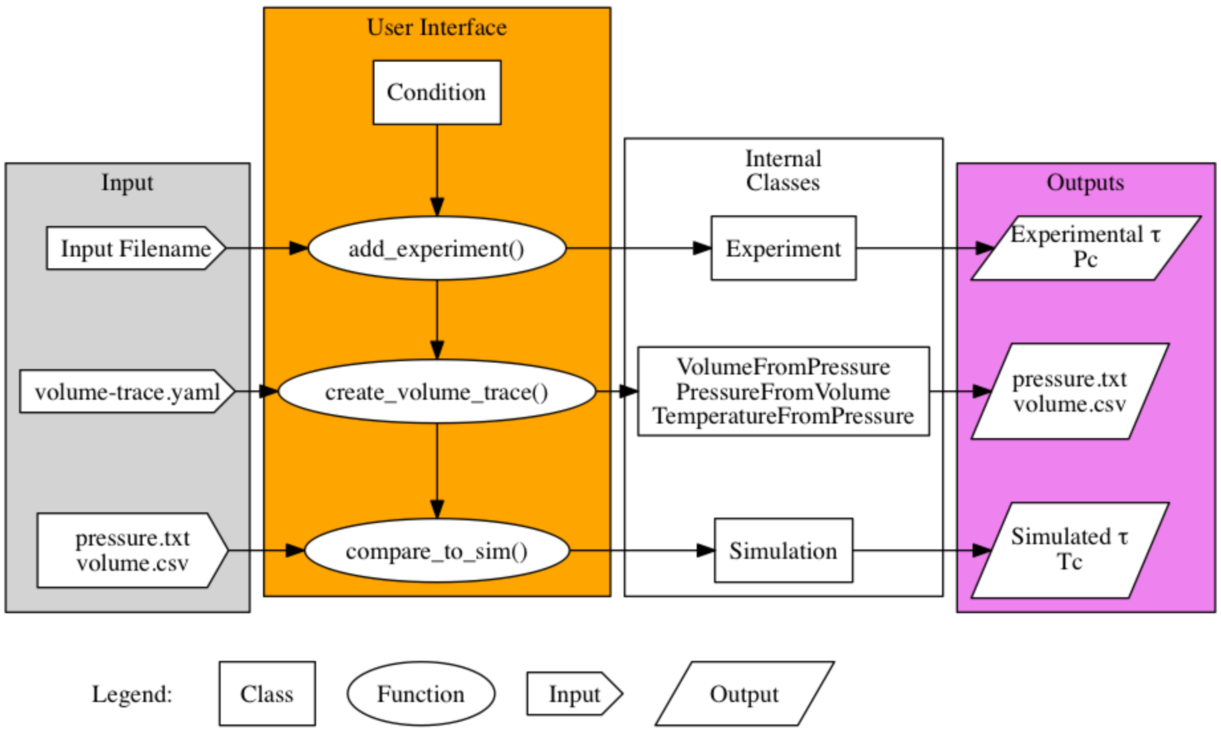
Modular Design

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



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Scientific Python Software

- SciPy for filter construction and convolution (`fftconvolve` was ~100x faster than NumPy's `convolve`)
- Cantera (https://github.com/Cantera/cantera) to calculate thermodynamic information about the reactor
- Matplotlib for plots
- Documentation is available online (http://bryanwweber.github.io/UConnRCMPy/), generated by Sphinx

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Demo

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jupyter demo Last Checkpoint: Yesterday at 12:54 PM (unsaved changes)

File Edit View Insert Cell Kernel Help | Python 3

Markdown CellToolbar

SciPy 2016 UConnRCMPy demo

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

```
Using matplotlib backend: MacOSX
```

Out[1]:
```
['.DS_Store',
 '.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']
```

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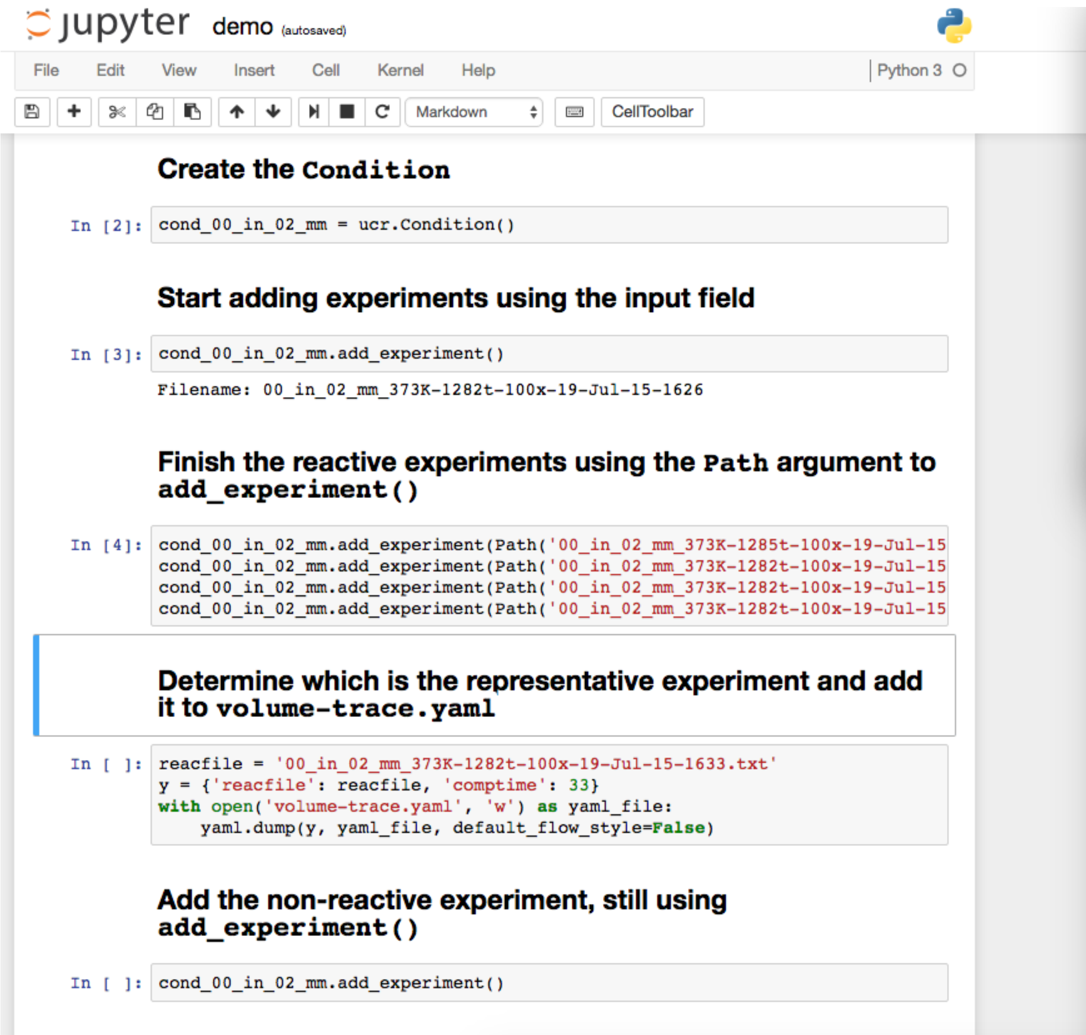

jupyter demo (autosaved)
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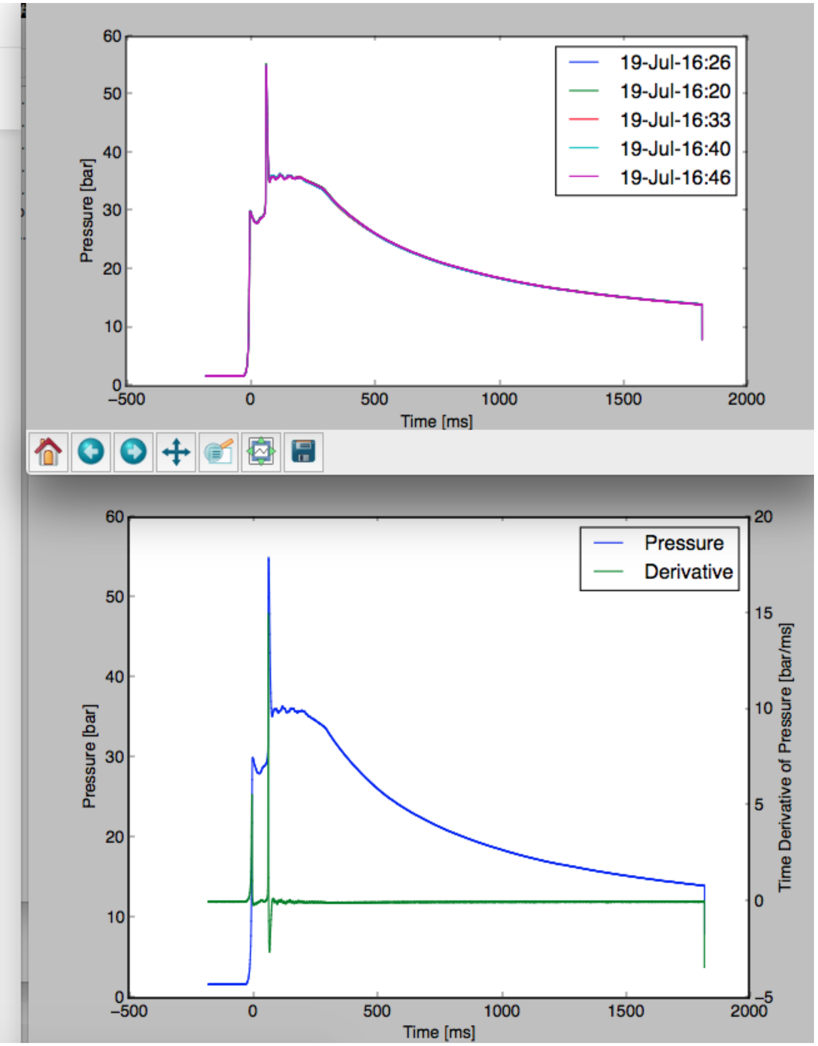
Python 3
Markdown
CellToolbar
Create the Condition
In [2]: cond_00_in_02_mm = ucr.Condition()
Start adding experiments using the input field
In [3]: cond_00_in_02_mm.add_experiment()
Filename: 00_in_02_mm_373K-1282t-100x-19-Jul-15-1626
Finish the reactive experiments using the Path argument to add_experiment()
In [4]: cond_00_in_02_mm.add_experiment(Path('00_in_02_mm_373K-1285t-100x-19-Jul-15
cond_00_in_02_mm.add_experiment(Path('00_in_02_mm_373K-1282t-100x-19-Jul-15
cond_00_in_02_mm.add_experiment(Path('00_in_02_mm_373K-1282t-100x-19-Jul-15
cond_00_in_02_mm.add_experiment(Path('00_in_02_mm_373K-1282t-100x-19-Jul-15
Determine which is the representative experiment and add it to volume-trace.yaml
In [ ]: reacfile = '00_in_02_mm_373K-1282t-100x-19-Jul-15-1633.txt'
y = {'reacfile': reacfile, 'comptime': 33}
with open('volume-trace.yaml', 'w') as yaml_file:
    yaml.dump(y, yaml_file, default_flow_style=False)
Add the non-reactive experiment, still using add_experiment()
In [ ]: cond_00_in_02_mm.add_experiment()



Pressure [bar]
Time [ms]
19-Jul-16:26
19-Jul-16:20
19-Jul-16:33
19-Jul-16:40
19-Jul-16:46
Pressure
Derivative
Time Derivative of Pressure [bar/ms]

fx Time

	A	B	C	D	E	F	G	H	I	J	K	L
1	Time	P0	T0	Pc	Tig	First Stage	Tc	in Spacers	mm Shims	Right Tank		
2	1307	878	413	29.92496204	11.88		895.5559595	2	0	O2	252	
3	1314	880	413	29.96528205	11.68		903.4760968	2	0	N2	2399	
4	1322	880	413	30.04718894	11.58		896.9368688	2	0	DME	2399	
5	1329	880	413	30.00451748	11.67		897.6781982	2	0	C3H8	2500	
6	1336	880	413	29.99434871	11.44		894.7526087	2	0	Pd	100	
7										Ta	23.3	
8				Mean	11.65							
9				Std. Dev.	0.16							
10				%	1.38							
11												

jupyter demo Last Checkpoint: 9 minutes ago (autosaved)

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

In [8]:
```python
nonrfile = 'NR_00_in_02_mm_373K-1278t-100x-19-Jul-15-1652.txt'
y = {**y, 'nonrend': 400, 'reacend': 80, 'nonrfile': nonrfile}
with open('volume-trace.yaml', 'w') as yaml_file:
    yaml.dump(y, yaml_file, default_flow_style=False)
```

Then we need to create the volume trace used for modeling

In [9]:
```python
cond_00_in_02_mm.create_volume_trace()
```

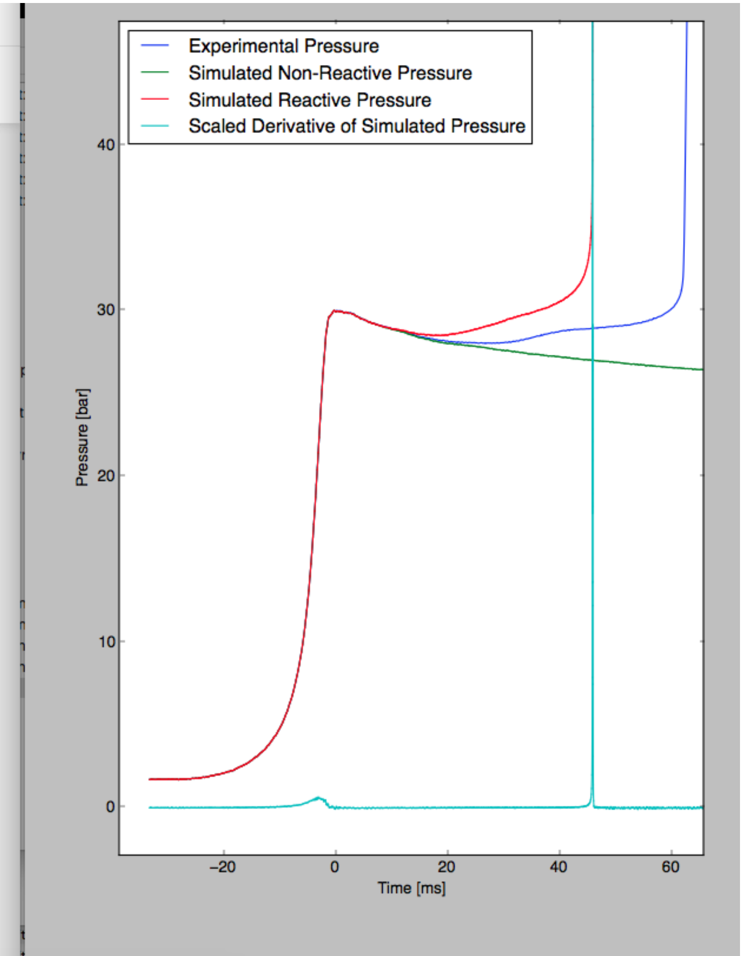
Then run the simulation to determine T_C

In [12]:
```python
cond_00_in_02_mm.compare_to_sim(run_reactive=True, run_nonreactive=True)
```

```
Are you sure you want to overwrite the nonreactive simulation? Input y or n: n
Nothing was done
Are you sure you want to overwrite the reactive simulation? Input y or n: y
759     46.116253
```

In [13]:
```python
os.listdir('.')
```

Out[13]:
```
['.DS_Store',
 '.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',
 'volume-trace.yaml',
 'volume.csv']
```



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Future Work

- Automatic calculation of optimal low-pass filter cutoff frequency
- Automatic calculation of optimal moving-average smoothing filter width
- Improved detection of the EOC
- Unit testing!
- See https://github.com/bryanwweber/UConnRCMPy/issues

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Acknowledgements

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