Open-Software Tools for the Analysis of Electrochemical Impedance Spectra

AiMES ECS Data Science Showcase

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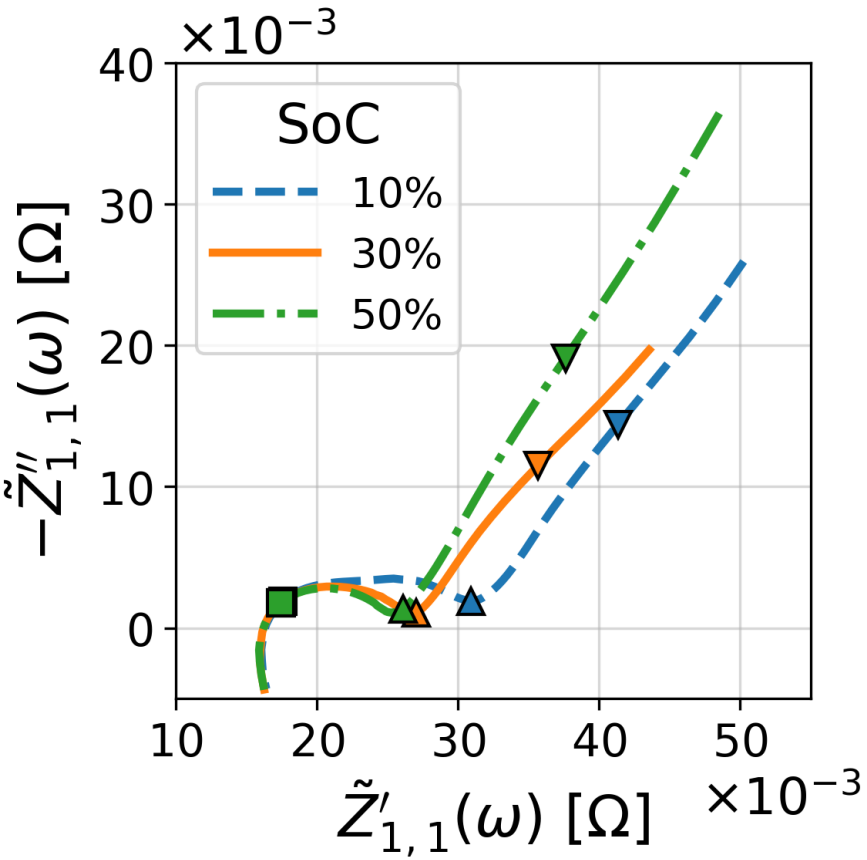
Goal: extract *physically meaningful* and *reliable* insights from data



- Battery health
- Relative impact of kinetics/transport
- Quantitative parameters
- ...

Murbach, M. D. et al. *J. Electrochem. Soc.* 165, A2758 (2018)

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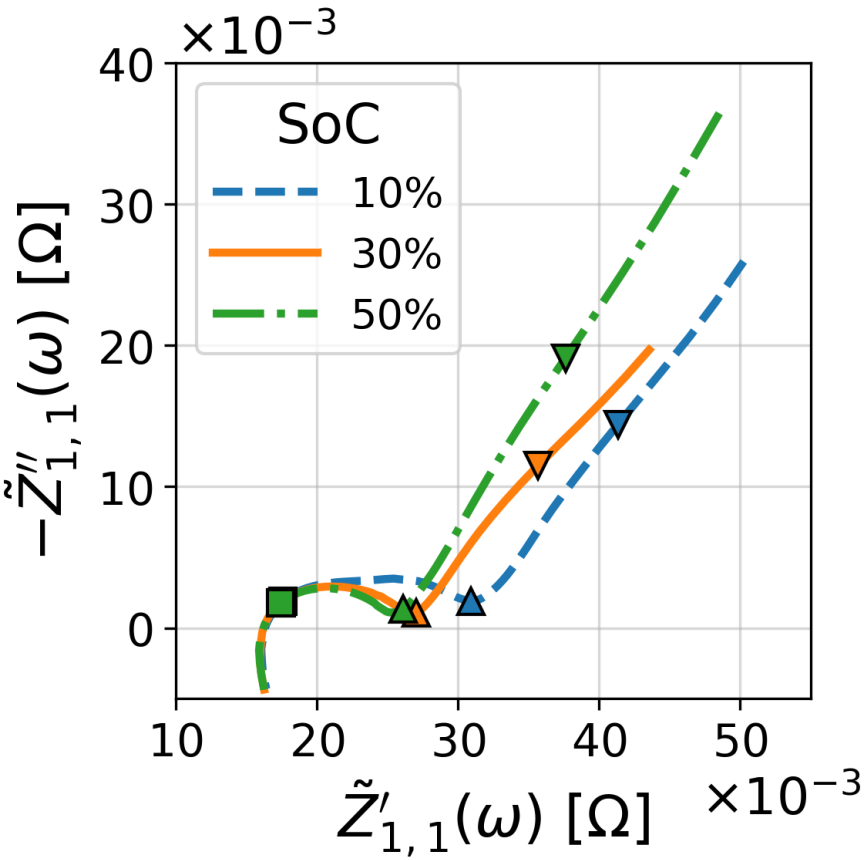

Current analysis options:

- Potentiostat software
- Proprietary 3^{rd} party software
- Code written in individual labs

Metrohm Autolab

ZView®

EIS Spectrum Analyser

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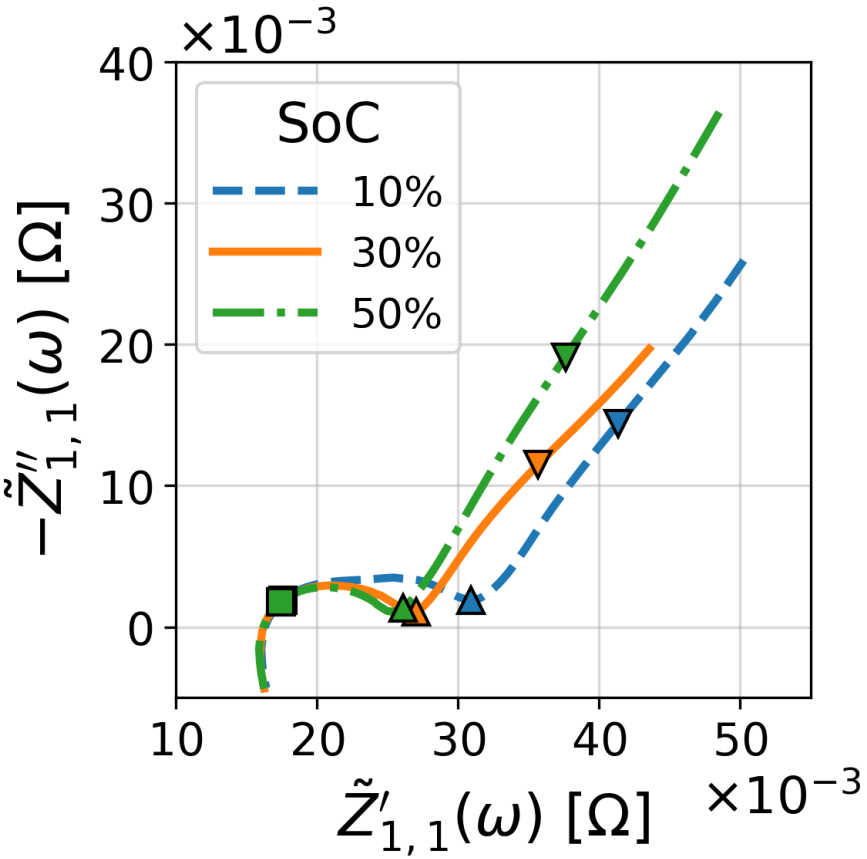

Current analysis options:

Metrohm Autolab

ZView®

EIS Spectrum Analyser

- Typically clunky to use
- Proprietary/hidden algorithms (cant reproduce!)
- Difficult to share and improve

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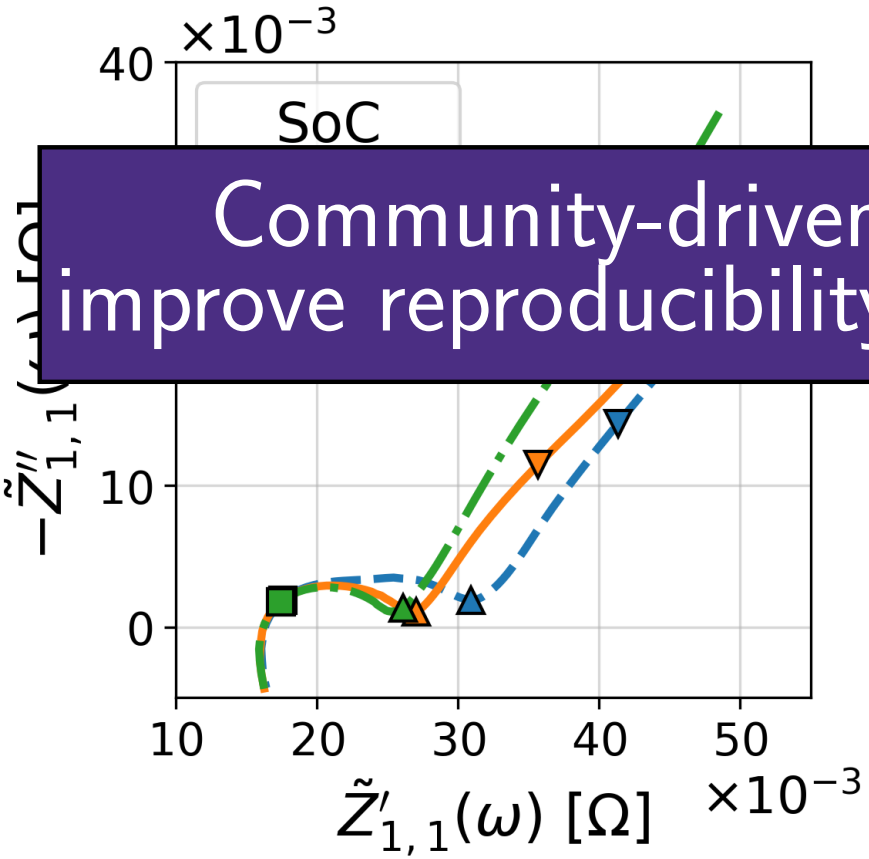

Current analysis options:

Community-driven, open-source tools improve reproducibility and accelerate science

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Murbach, M. D. et al. *J. Electrochem. Soc.* 165, A2758 (2018)

What will the future of impedance analysis look like?

- Fast, **reproducible** analysis of impedance spectra
- Easy-to-use software that encourages **best practice**
- **Community-driven** toolkit grows with improved methods for interpretation and analysis

An example: Scikit-learn has made high-quality machine learning available to all

machine learning made easy-to-use

- Easy to apply and compare different models, open and powerful enough to accomplish real tasks
- The key is the *community-driven api*

1^{st} steps: Python package + web-based GUI

impedance.py

```
In [1]: import matplotlib.pyplot as plt
        import numpy as np

        from impedance.circuits import CustomCircuit

In [2]: # read data
        data = np.genfromtxt('../../../data/exampleData.csv', delimiter=',')

        frequencies = data[:,0]
        Z = data[:,1] + 1j*data[:,2]

        frequencies = frequencies[np.imag(Z) < 0]
        Z = Z[np.imag(Z) < 0]

In [3]: circuit = CustomCircuit(initial_guess=[.01, .005, .1, .005, .1, .001, 200], circuit='R_0-p(R_1,C_1
        )-p(R_1,C_1)-W_1/W_2')

        circuit.fit(frequencies, Z)

        print(circuit)

        ------------------------------
        Circuit: None
        Circuit string: R_0-p(R_1,C_1)-p(R_1,C_1)-W_1/W_2
        Algorithm: leastsq
        Fit: True
        Fit parameters:
                R_0 = 1.65e-02
                R_1 = 8.77e-03
                C_1 = 3.28e+00
                R_1 = 5.31e-03
                C_1 = 2.32e-01
                W_1 = 6.37e-02
                W_2 = 2.38e+02

        ------------------------------
```

ImpedanceAnalyzer

Murbach, M. D. et al. *J. Electrochem. Soc.* 165, A297 (2018)

impedance.py demo

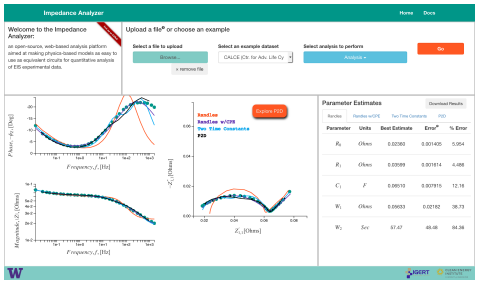
https://github.com/ECSHackWeek/impedance.py

ImpedanceAnalyzer demo

https://github.com/mdmurbach/ImpedanceAnalyzer

Murbach, M. D. et al. *J. Electrochem. Soc.* 165, A297 (2018)

Moving from beta to ImpedanceAnalyzer v1.0



- Login/save data and settings
- Additional physics-based datasets
- Implement confidence interval estimation and visualization
- Drag-n-drop circuit creation
- Desktop vs. web application

Expanding usability and features of impedance.py

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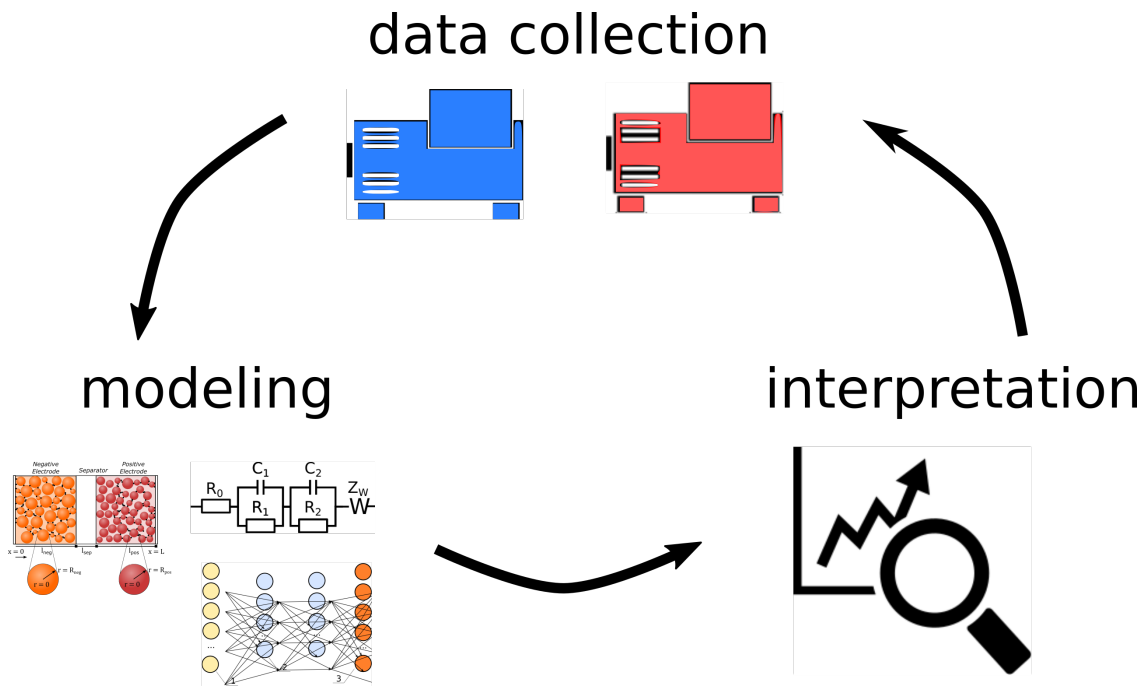
        ------------------------------
```

- Incorporate interactive visualizations
- Additional equivalent circuit and physics-based models and elements
- Improve initialization of smart parameter guesses
- Improve data validation methods
- ...

longer-term vision:

open API for data, analysis, and interpretation pipeline



Thank you!

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- Prof. Dan Schwartz
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