5. Electrochemical energy storage systems (ORNL, UT Austin)

Research thrusts: *Fast & reliable solution of multiphysics/multiscale problems; Validation, adaptation, and management of models*

Research sub-thrusts: *Accurate, robust discretizations; Error estimation; Inadequacy modeling*

ORNL developed software to support the research in electrochemical energy storage systems. The code is open source, available on github. It provides a straightforward API that aligns well with real-world electrochemical experiments and is designed to ease development and testing of numerical models for energy storage devices. In collaboration with UT Austin, ORNL examined the inadequacy of lower-fidelity equivalent circuit models for predicting the behavior of the supercapacitor double-layer. For that purpose, we investigated various techniques to characterize the electrochemical behavior of storage systems which lead us to perform full impedance spectroscopy analysis on our high-fidelity models (a unique capability!). Fig. 9 plots the frequency response of the finite-element model next to a simple resistor-capacitor equivalent circuit, demonstrating that the equivalent circuit model is unable to capure the higher frequency behavior of supercapacitors.

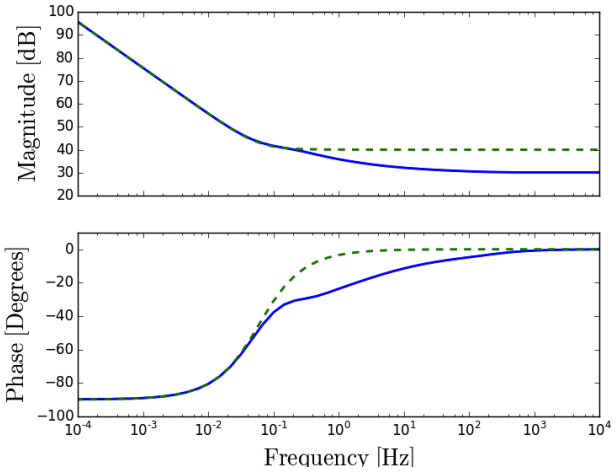

Figure 9: Electrochemical impedance spectra over a representative range of frequencies for a higher-fidelity model (solid blue line) and its equivalent cicuit (dashed green).