Modeling Inadequacy in Hierarchical Models of Supercapacitors

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Development of inadequacy representations for simple zero-dimensional models of super-capacitors was started with input from John Turner (PI) and Damien Lebrun-Grandie at Oak Ridge. The model problem being pursued is the up-scaling of a one-dimensional linear model that does not include Faradaic effects. The analytic solution of this "high fidelity" model is available and shows that an exact zero-dimensional non-Markovian model can be derived in terms of a history integral. This is impractical in general, so in this case the stochastic inadequacy representation needs to account for the incomplete history information available to the low-fidelity model. This suggests a formulation in terms of an auxiliary stochastic ordinary differential equation representing an uncertain history, and the challenge is to constrain it to be consistent with plausible system state histories. The cell voltage V_{cell} for applied electrical current to the super-capacitor cell is taken into account as the quantity of interest (QoI). We used information from residual associated with solution of LF model of overpotential evolution $\eta_{LF}(\xi, \tau)$ to estimate error in QoI, $\epsilon_{QoI} = V_{cell}(\eta_{HF}) - V_{cell}(\eta_{LF})$, without having to solve HF model. Figure (1) shows the spatial and temporal evolution of η_{LF} during a cyclic charge-discharge, a common technique used to test the performance and cycle-life of energy storage devices, and the corresponding error in QoI.

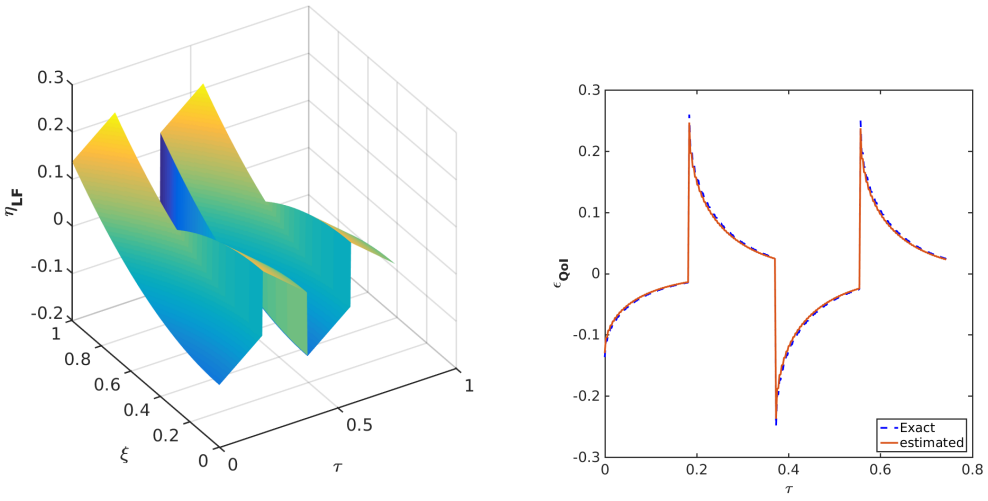

Figure 1: (left) Solution of LF model η at different normalized time τ and space ξ; (right) comparison of the estimated and exact error in QoI using LF and IF models $\epsilon_{QoI} = V_{cell}(\eta_{HF}) - V_{cell}(\eta_{IF})$.