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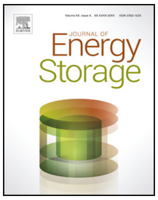

Simulation of thin-film battery response to periodic loading by a transition matrix approximation using boundary and nonlinearity error analysis

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ABSTRACT

Simulating repeating loading events on dynamic systems can be challenging when large timescale disparities exist coupled with aperiodic effects. Batteries driving switched/pulsed loads represent one such situation. Large timescale disparity can be experienced by solid-state batteries driving switching microactuators or microelectronics, due to extremely short transient response times of microscale systems relative to some of the battery's own dynamics. Projecting state changes over a long series of fast-timescale loading events using a transition matrix approach was shown previously to significantly reduce numerical expense of simulation compared to full modeling. Here we develop an approach for further accelerated simulation of a battery driving a microelectromechanical system (MEMS) actuator that quantifies errors and addresses overhead expenses in projecting battery states across multiple fast events. This is done with a definition of system states that allows efficient transition matrix generation, and an analysis of key errors associated with projection. This error analysis enables targeted modification to the transition matrix during projection. A case study explores these modeling approaches in a capacitively loaded, battery usage scenario of a piezoelectrically-driven microrobot where the proposed improvements reduce the numerical cost (function calls) by over 44x from the prior approach. Conditions for further simplified modeling are discussed.

1. Introduction

Thin-film solid-state batteries provide a convenient power source for many small engineered systems, particularly microsystems based on integrated circuit and micro-electromechanical system (MEMS) technologies. In many such systems, battery loading occurs as repeated short-duration transient events, such as to drive microactuators or switching electronics in periodic operation. Individual loading events may occur over time periods of just a few microseconds, given the high bandwidths of associated electrical or electromechanical components, while complete battery discharge may occur over several hours. This vast disparity in timescales can make high-fidelity simulation of battery behavior based on physics-based partial differential equation models, very challenging. Nonetheless, such simulation can be beneficial for understanding influences of system-level design choices (i.e. loading frequency and component sizes) on anticipated battery performance or assessing the accuracy of simplified reduced-order or equivalent circuit battery models. This paper thus proposes a strategy for efficiently simulating repeated transient loading effects on a solid-state battery model using a numerically-identified state-transition matrix approach, and illustrates how error analysis of the numerical method can be used to further improve simulation efficiency and/or accuracy.

In general, modeling of power/battery systems can be an important tool for improving design and control, and has been performed in a variety of ways including electrochemical [1–3] and equivalent circuit modeling [4,5]. Different approaches for model reduction have also been attempted to make the system easier to handle. For example, Santhanagopalan et al. [6] compares model reduction strategies for lithium-ion batteries with porous electrodes, for full discharge cycling; Kim and Qiao [7] present a hybrid

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Nomenclature

Symbol and description

$\mathbb{Y}$	Normalized lithium concentration, subscript denotes positive electrode (+) or electrolyte (e)
$\mathbb{T}$	Normalized time
$\mathbb{X}$	Normalized spatial location in positive electrode
$\mathbb{D}$	Normalized diffusion coefficient
$\mathbb{I}$	Normalized current
$\mathbb{V}$	Normalized voltage, subscripts denote various locations in the battery
α_a	Anodic charge transfer coefficient subscripts denote positive or negative electrode
$\mathbb{U}$	Normalized open circuit potential
$\mathbf{A}, \mathbf{B}$	Finite difference matrices
$\mathbf{r}$	Finite difference vector containing boundary condition information
p, r, q, s, C	Variables used for finite difference matrix formulation
h	Finite difference element length
τ	Finite difference time step length
$\mathbf{\Phi}$	Transition matrix
$\mathbf{B}^*, \mathbf{r}^*$	Modified matrix/vector accounting for boundary concentrations
$\mathbf{E}$	Error

model that combines simplicity with nonlinear effects with demonstration on a limited number of pulses during discharge; and Afshar et al. [8] uses a reduction method to address the boundary conditions transforming them to differential equations through linearization.

In microscale applications, it is also important to understand the usage of battery capacity due to the limited payload and footprint available. The effects of intermittent loading on different types of batteries have been discussed in the literature with varying opinions [9–11]. Additionally, from a computational perspective, merely modeling the individual loading event dynamics can be numerically expensive. Fully modeling this problem, when coupled with the many loading events (potentially millions), can be impractical.

One example of intermittent battery loading for MEMS devices, to be the focus of the case study in this paper, is that of switched piezoelectric or electrostatic MEMS actuation, both of which act as capacitive loads in terms of electrical behavior. This type of loading, especially when coupled with power electronics' dynamics, can have effects on multiple timescales as is shown in the conceptual schematics of a microrobot in Fig. 1 based on work in [12]. The authors have previously shown experimentally that useful battery lifetime when driving a capacitive load can have complex dependence on details of switching frequency, load capacitance, and various circuit current and switching losses [13]. From a modeling perspective, the authors have also shown that resulting battery behavior can be captured through adaptation of existing thin-film electrochemical models [2,3] through inclusion of additional switching and loading effects [14]. However, the accumulation of repeated individual loads created a dual-timescale problem when analyzing battery behavior over a complete discharge. In the earlier work, this was addressed by systematically perturbing system states, or changes in Li concentration at discretized points. In that manner, a numerical Jacobian or "transition matrix" could be developed describing changes in the system states over one fast-dynamic event. That transition matrix then could be used to approximate (or "project" over) multiple fast-dynamic events. This permitted simulation of battery discharge to be greatly accelerated, but simulation remained extremely computationally expensive and dependent on available hardware for parallelizing transition matrix development due to the large number of perturbations required. Furthermore, sources of accumulated error between the full model and accelerated simulation were not readily identifiable.

From a numerical methods perspective, the modeling and simulation of systems with disparate timescales is known to be challenging. Nonetheless, different approaches can be used depending on the specifics of the problem being analyzed. Engstler and Lubich presented an extrapolation approach where aspects of the problem are inactivated during portions of the extrapolation to reduce computation [15]. Constantinescu and Sandu extended this for "extrapolated explicit and implicit compound multirate steps" [16]. Roychowdhury discusses analysis of multiple time scale circuits by using different time variables [17]. Edwards shows an example approach with a heat conduction problem of two timescales [18]. A broad discussion on the topic of multiple timescales is given in [19].

Due to several features common to electrochemical battery modeling, the implementation approach of these traditional multi-scale methods may not be directly applicable. These aspects include: variable coefficients (seen in the concentration dependency of the diffusion coefficient), multiple timescale boundaries (slow evolving open circuit potential and fast switching dynamics), Neumann-type boundaries (positive electrode concentration), non-linear algebraic constraint of the boundary (exponential form of the Butler-Volmer equations), and the fact that the slow dynamics are produced due to accumulation of repeated fast dynamic events. While this does not preclude the possibility of adapting the above methods to the thin-film battery simulation problem examined here, this paper focuses on transition matrix methods as introduced above.

Here, we propose the use of intrinsic dynamics and numerical error analysis to model thin-film solid-state battery behavior over repeated fast timescale loading events in a computationally efficient form. First, we review the basic electrochemical battery model applied in previous work. Then, we describe how to directly compute a transition matrix for states of the discretized electrochemical model over fast timescale events using lithium

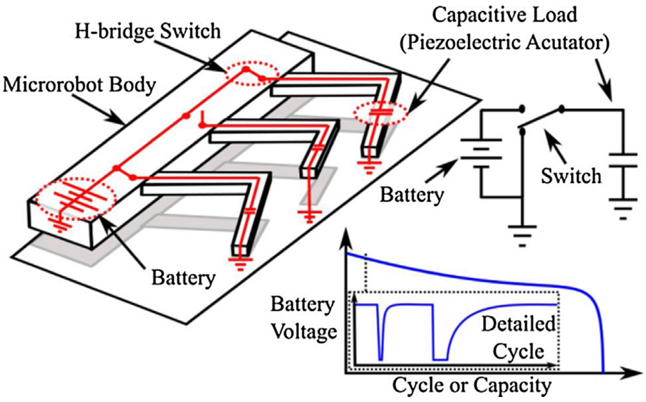

Fig. 1. MEMS micro-robot [12] switching and actuation schematics. A micro-robot schematic with a simplified equivalent circuit overlaid in red on the robot body is shown. A simplistic battery switching schematic, with an H-bridge (represented schematically as a simple single-pole double-throw switch) is shown, and similar simplistic switching was used in the case study here. A sample battery discharge profile is shown with a representative single capacitor charge cycle profile. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)