An Adaptive Reduced-Order-Modeling Approach for Simulating Real-Time Performances of Li-Ion Battery Systems

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In this work, a reduced-order-modeling (ROM) approach is introduced to simulate a battery system with multiple cells. The ROM is described by only two state variable equations and several explicit expressions. While running a stand-alone pseudo-2D (P2D) model by the nonlinear state variable modeling (NSVM) algorithm at a specified current, several parameters can be estimated through the NSVM procedure; and with these parameters, the cell voltage under additional current perturbations can be computed approximately by the ROM. This modeling scheme was tested for a 24P battery module in a co-simulation process: the stand-alone P2D model is solved at the battery-average current to estimate certain parameters to share with its ROM, then the ROM is implemented to evaluate the voltage response of each cell at its respective cell current. The ROM shows excellent accuracy and a much higher speed than the full-order-model with P2D models used for each cell.

The battery management system (BMS) plays a crucial role in electrical vehicles (EV). During a standard vehicle development cycle, in-loop simulation is a useful technique to test and verify complex real-time embedded systems.1-3 To conduct in-loop simulation, the embedded system to be tested is connected to a mathematical representation of all related dynamic systems, because this arrangement lowers cost and improves safety as compared with using the real system. The mathematical representation interacting with embedded system is referred as “plant simulation”. For the BMS software development, the plant simulation is performed by system-level battery models while the corresponding embedded system includes certain battery control and management algorithms. Therefore an accurate plant model for the battery system is vital for a successful BMS design. Besides accuracy, the plant battery model is also expected to work under high frequency inputs with noise and generate real-time output signals at low computational costs.

The pseudo-2D (P2D) model developed by Fueller et al.4 is a physical model that can be used to provide reliable predictions for the transport and electrochemical phenomena in Li-ion cells. However, it is still difficult to use the P2D model in plant simulation. The first challenge is the numerical issues in solving the nonlinear partial-differential-equations (PDEs) contained in the P2D model at high-frequency inputs. During practical driving modes, the power requests from the powertrain to the EV battery change very quickly with time, and the currents and voltages are processed as discrete-time electrical signals. Most multi-physics PDE solvers (e.g., COMSOL) are designed to model continuous-time processes (e.g., constant current) and are slow for high-frequency simulation cases. Another challenge is the high computational costs to scale up the P2D model from cell-level to pack-level. A single-cell P2D model normally includes more than 100 discretized state variables even using a very coarse mesh. To meet the high power and energy demands, typical EV battery packs are made of hundreds to thousands of cells with extra connecting auxiliaries. Most of these EV packs employ a “mPnS” connection pattern or even an internal resistance component.13,14 The parameters in these ROMs need to be validated from the results of a rigorous model or directly from test data. For example, the RC components in an equivalent circuit can be evaluated by fitting the high-power-pulse-cycle (HPPC) profiles through various state-of-charge (SOC) and temperature ranges. These ROM approaches show poor robustness when working outside the SOC and temperature windows where the parameters can be effectively validated. For example, the RC components always fail for continuous discharges at SOC<10%, because the nonlinear mass transfer limitations in these operation conditions cannot be captured during the HPPC validation procedures.

The purpose of this work is to introduce an adaptive ROM approach developed based on our NSVM algorithm. We found that while solving a P2D cell model using NSVM with certain instantaneous current input, some operators can be further utilized to approximate the voltage responses when different current perturbations are added to the

Manuscript submitted October 2, 2017; revised manuscript received November 10, 2017. Published November 24, 2017.

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system. For a nPrS battery configuration, the average current is calculated by dividing the total pack current by the parallel number \( m \), and the deviation between the individual cell currents and the average current can be regarded as a current perturbation. Therefore, by feeding the average current to a stand-alone P2D model at each time instance, a ROM can be derived from the NSVM procedure and then can be applied to calculate the voltage responses of each individual cell. As this workflow is implemented with real-time input signals, the ROM parameters can also be optimized on a real-time basis to obtain improved accuracy. The details for this mathematical method are shown in the following sections.

### Mathematical Model

Newman’s P2D model equations are given in Appendix A, including the illustrative schemes (Figure A1), governing equations (Table A1), and expressions for some physical variables (Equations A1 through A3).

#### General form of reduced-order model (ROM).

In the P2D model, the cell voltage is defined as equal to the solid phase reference potential for cathode:

\[
V_{\text{P2D}} = \phi_s^{\text{ref}}
\]

where \( V_{\text{P2D}} \) is the cell voltage estimated by P2D model at a specific current \( I \), and \( \phi_s^{\text{ref}} \) is the solid phase potential defined at the boundary of cathode current collector (\( x = l_a + l_s + l_p \)). In this work, the variable \( \phi_s^{\text{ref}} \) is split into three terms: the equilibrium voltage \( U_{\text{eq}} \), the electrical over voltage \( V_e \), and the diffusional over voltage \( V_d \):

\[
\phi_s^{\text{ref}} = U_{\text{eq}} + V_e + V_d
\]

and therefore \( V_{\text{P2D}} \) is given by:

\[
V_{\text{P2D}} = U_{\text{eq}} + V_e + V_d
\]

Let \( \Delta I \) stand for a small perturbation in the current, and the cell voltage at current \( I' = I + \Delta I \) will be estimated using a reduced order model (ROM) as follows:

\[
V_{\text{ROM}} = U'_{\text{eq}} + V_e' + V_d'
\]

where \( V_{\text{ROM}} \) is the voltage estimated by the ROM. \( U'_{\text{eq}}, V_e', \) and \( V_d' \) are respectively the equilibrium voltage, electrical over voltage, and diffusional over voltage estimated at the current \( I' = I + \Delta I \) and \( I' \) take positive values for charge and negative values for discharge. The derivation of these variables will be given later.

#### Equilibrium voltage.

According to Reference 9, the dimensionless concentration of Li ions in active material particle, \( \theta_{\text{avg}} \), is governed by the following equation:

\[
\frac{d\theta_{\text{avg}}}{dt} = \frac{-3j_i}{R_iF_c}\]

where \( c_{\text{max}} \) is the maximum Li concentration in the active material, \( F \) is the Faraday’s constant, \( j_i \) is the local electrochemical current density, \( R_i \) is the radius of active material particle, and \( t \) is time. The electrode average concentration of Li ions through anode and cathode domains, \( \theta_a \) and \( \theta_p \), are defined by:

\[
\theta_a = \frac{1}{l_a} \int_{l_0}^{l_a} \theta_{\text{avg}} dx \quad \theta_p = \frac{1}{l_p} \int_{l_{a+s}}^{l_a+l_s+l_p} \theta_{\text{avg}} dx
\]

where \( l_a, l_s, \) and \( l_p \) are respectively the thickness of anode, separator, and cathode. The overall charge conservation in the anode and cathode domains are respectively given by:

\[
\int_{l_0}^{l_a} a_{s,a} j_a dx = -\frac{I}{A_c} \int_{l_{a+s}}^{l_a+l_s+l_p} a_{s,p} j_a dx = \frac{I}{A_c}
\]

where \( a_{s,a} \) and \( a_{s,p} \) are respectively the specific surface area of anode and cathode, and \( A_c \) is the coating area of the cathode. By substituting Equation 5 into 6 and applying Equation 7, the governing equations for \( \theta_a \) and \( \theta_p \) can be derived as follows:

\[
\frac{d\theta_a}{dt} = \frac{3I}{A_c a_{s,a} R_i F_c c_{s,max}} \quad \frac{d\theta_p}{dt} = \frac{3I}{A_c a_{s,p} R_i F_c c_{s,max}}
\]

where the subscripts “a” and “p” respectively denote anode and cathode. When a cell is fully equilibrated, there are no concentration gradients in the solid and electrolyte phases, and the dimensionless Li ion concentration in anode and cathode particles are uniform and respectively equal to \( \theta_a \) and \( \theta_p \). Therefore, the equilibrium cell voltage is calculated by:

\[
U_{\text{eq}} = U_p (\theta_p) - U_a (\theta_a)
\]

where \( U_a \) and \( U_p \) are half-cell open circuit potentials for anode and cathode whose profiles are presented in Appendix A. The following constraint for \( \theta_a \) and \( \theta_p \) can be derived from Equation 8:

\[
a_{s,a} R_i c_{s,max} \frac{d\theta_a}{dt} + a_{s,p} R_i c_{s,max} \frac{d\theta_p}{dt} = 0
\]

Equation 10 can also be expressed as follows by integrating with time:

\[
a_{s,a} R_i c_{s,max} \theta_a + a_{s,p} R_i c_{s,max} \theta_p = C_0
\]

where \( C_0 \) is a constant which can be evaluated at initial time \( t = 0 \):

\[
C_0 = a_{s,a} R_i c_{s,max} (t = 0) + a_{s,p} R_i c_{s,max} \theta_p (t = 0)
\]

therefore \( \theta_p \) is a linear function of \( \theta_a \):

\[
\theta_p = C_0 - \frac{a_{s,a} R_i c_{s,max}}{a_{s,p} R_i c_{s,max}} \theta_a
\]

According to Equations 9 and 13, the equilibrium cell voltage can be expressed as a single variable function of \( \theta_a \):

\[
U_{\text{eq}} = F (\theta_a) = U_p (\theta_a) - U_a (\theta_a)
\]

For the ROM, the following equations are used to evaluate \( U'_{\text{eq}} \) at current \( I' = I + \Delta I \):

\[
\frac{d\theta_a}{dt} = \frac{3I'}{A_c a_{s,a} R_i F_c c_{s,max}}
\]

where \( \theta_a' \) is the anode average dimensionless Li ion concentration for current \( I' = I + \Delta I \). Next, we need to express Equations 15 and 16 in state-space form; from discretized time instance \( t[k - 1] \) to \( t[k] = t[k - 1] + \Delta t \), variable \( \theta_a' \) can be evaluated by the forward time-integral method:

\[
\theta_a' [k] = \theta_a' [k - 1] + \frac{3I'}{A_c a_{s,a} R_i F_c c_{s,max}} \Delta t
\]

where “[k]” and “[k - 1]” in variables stand for values at time instances \( t[k] \) and \( t[k - 1] \). Therefore \( U'_{\text{eq}} \) is computed at each discretized time instance:

\[
U'_{\text{eq}} [k] = F \left( \theta_a' [k] \right)
\]
Electrical over voltage.—According to Equation 58 of Reference 9, through a linearized Butler-Volmer equation, the reference solid phase potential can be approximated by

\[ \Phi_{S}^{ref} = u_B + z_n I_B \]  

where \( \Phi_{S}^{ref} \) is the approximated reference solid phase potential, and \( I_B = -\frac{J}{J_0} \) is the inward current density at the cathode/current collector boundary \((s = l_c + l_I + l_p)\). The expressions for \( u_B \) and \( z_n \) are given in Reference 9. The Butler-Volmer equation turns from hyperbolic to linear as the current density goes close to zero, which means \( \Phi_{S}^{ref} = \Phi_{S}^{ref} \) when \( I \to 0 \). Furthermore, it can be shown from Equation 19 that \( \Phi_{S}^{ref} = u_B \) as \( I \to 0 \), therefore \( \Phi_{S}^{ref} = u_B \) for currents close to zero. As discussed above, \( u_B \) stands for \( \Phi_{S}^{ref} \) evaluated at zero current. According to Reference 9, the value of \( u_B \) only depends on the concentrations of solid and electrolyte phases; therefore at time instance \( k \), the value for \( u_B \) can be expressed as function of discretized solid/electrolyte concentrations:

\[ u_B[k] = \text{func} (\mathbf{x}[k]) \]  

where \( \mathbf{x}[k] \) is the vector for the discretized concentration variables. In our NSVM, the concentration states are updated by the forward time integral approach:

\[ \mathbf{x}[k] = \Delta \mathbf{A}[k-1] + \Delta \mathbf{B}[k-1] \]  

where \( \mathbf{A}, \mathbf{A}', \) and \( \mathbf{B} \) are matrix operators, and \( \mathbf{d}[k-1] \) is the source term vector at \( t[k-1] \). The values for \( \mathbf{d}[k-1] \) are calculated from \( I[k-1] \) but have no dependency on \( I'[k] \); therefore by analyzing Equations 20 and 21, the value for \( u_B[k] \) does not depend on \( I[k] \):

\[ \frac{\partial u_B[k]}{\partial I'[k]} = 0 \]  

At each time instance, the electrical over voltage is defined as the difference between \( \Phi_{S}^{ref} \) and \( u_B \):

\[ V_e[k] = \Phi_{S}^{ref}[k] - u_B[k] \]  

and at current \( I'[k] = I[k] + \Delta I \), the electrical over voltage \( V_e \) can be approximately expressed as follows:

\[ V_e[k] = V_e[k] + R_e[k] (I'[k] - I[k]) \]  

where \( R_e[k] \) is the instantaneous kinetic resistance of the cell given by:

\[ R_e[k] = \frac{\partial V_e[k]}{\partial I'[k]} \]  

According to Equations 22 and 23, \( R_e[k] \) can also be expressed as follows:

\[ R_e[k] = \frac{\partial \Phi_{S}^{ref}[k]}{\partial I'[k]} \]  

To calculate \( R_e[k] \), we start from Equations 79 and 81 in Reference 9 which can be written as follows when the Newton loop converges at time instance \( t[k] \):

\[ \mathbf{Jac} \begin{bmatrix} \frac{d \mathbf{j}}{d I'[k]} \\ \frac{d \Phi_{S}^{ref}[k]}{d I'[k]} \\ \frac{d \Phi_{S}[k]}{d I'[k]} \\ \frac{d I_B[k]}{d I'[k]} \end{bmatrix} = 0 \]  

where \( \mathbf{Jac} \) is the Jacobian matrix, \( \mathbf{j} \) is the vector for electrochemical current densities and \( \Phi_{S}^{ref} \) is the reference potential of the electrolyte. In Equation 27, variables \( \frac{d \mathbf{j}}{d I'[k]}, \frac{d \Phi_{S}^{ref}[k]}{d I'[k]}, \frac{d \Phi_{S}[k]}{d I'[k]}, \) and \( \frac{d I_B[k]}{d I'[k]} \) are all close to zero. The Jacobian matrix \( \mathbf{Jac} \) can be expressed blockwise as follow:

\[ \mathbf{Jac} = \begin{bmatrix} \mathbf{J}_1 & \mathbf{J}_2 \end{bmatrix} \]  

where \( \mathbf{J}_1 \) is the right-most column vector of matrix \( \mathbf{Jac} \) and \( \mathbf{J}_2 \) is the remaining part of \( \mathbf{Jac} \). Equation 27 can be rewritten as follows by substituting \( \mathbf{Jac} \) with \( \begin{bmatrix} \mathbf{J}_1 & \mathbf{J}_2 \end{bmatrix} \) and \( I_B \) with \( -\frac{J}{J_0} \):

\[ \begin{bmatrix} \frac{d \mathbf{j}}{d I'[k]} \\ \frac{d \Phi_{S}^{ref}[k]}{d I'[k]} \\ \frac{d \Phi_{S}[k]}{d I'[k]} \\ \frac{d I_B[k]}{d I'[k]} \end{bmatrix} \cdot \mathbf{J}_2 = -\frac{J}{J_0} d I'[k] = 0 \]  

Left-multiply Equation 29 with an operator \( [0 \ 0 \ \cdots \ 1] \begin{bmatrix} \mathbf{I} & \mathbf{J}_1 \end{bmatrix} \mathbf{y}^{-1} \mathbf{I} \) to derive:

\[ d \Phi_{S}^{ref}[k] = \begin{bmatrix} 0 & 0 & \cdots & 1 \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{J}_1 \end{bmatrix} \mathbf{y}^{-1} \mathbf{I} \begin{bmatrix} \mathbf{J}_2 \end{bmatrix} d I'[k] \]  

and according to Equations 26 and 30, the value for \( R_e \) can be calculated by:

\[ R_e[k] = \frac{\partial \Phi_{S}^{ref}[k]}{\partial I'[k]} = \begin{bmatrix} 0 & 0 & \cdots & 1 \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{J}_1 \end{bmatrix} \mathbf{y}^{-1} \mathbf{I} \begin{bmatrix} \mathbf{J}_2 \end{bmatrix} \]  

In state-space form, Equation 24 is written as:

\[ V_e'[k] = V_e[k] + R_e[k] (I'[k] - I[k]) \]  

Diffusional over voltage.—According to the definition in Equation 59 of Reference 9, \( u_B \) is not necessarily equal to \( U_{eq} \) as concentration gradients might exist unless the cell is fully stabilized. Therefore the diffusional over voltage \( V_d \) is defined as the difference between \( u_B \) and \( U_{eq} \):

\[ V_d = u_B - U_{eq} \]  

According to the above discussion, the diffusional over voltage \( V_d \) is determined by the mass transfer processes in solid and electrolyte phases, therefore we assume that \( V_d \) can be approximately described by the following dynamic model:

\[ \frac{d V_d}{d t} = \frac{V_d}{\tau_d} + \frac{k_d I}{\tau_d} \ (V_d = 0 \ at \ t = 0) \]  

where \( \tau_d \) and \( k_d \) are, respectively, the time constant and gain for the model. Rewrite Equation 34 into the following state space format:

\[ V_d[k] = b_1[k] V_d[k-1] + b_2[k] I[k-1] \ k = 1, 2, \cdots \]  

\[ V_d[0] = 0 \ I[0] = 0 \]  

where the parameters \( b_1[k] \) and \( b_2[k] \) are respectively expressed by:

\[ b_1[k] = \exp \left( -\frac{\Delta t}{\tau_d} \right) \quad b_2[k] = 1 - \exp \left( -\frac{\Delta t}{\tau_d} \right) k_d \]  

In Equation 35, \( b_1[k] \) and \( b_2[k] \) can be regarded as parameters in a linear model:

\[ \mathbf{y}[k] = \mathbf{N}[k] \mathbf{b}[k] \]  

where the dependent variable vector \( \mathbf{y}[k] \) is defined as follows:

\[ \mathbf{y}[k] = \begin{bmatrix} V_d[1] \\ V_d[2] \\ \vdots \\ V_d[k] \end{bmatrix} \quad (k = 1, 2, \cdots) \]  

The independent variable matrix \( \mathbf{N}[k] \) is defined as follows:

\[ \mathbf{N}[k] = \begin{bmatrix} 0 & 0 \\ V_d[1] & I[1] \\ \vdots & \vdots \\ V_d[k-1] & I[k-1] \end{bmatrix} \quad (k = 1, 2, \cdots) \]  

and the parameter vector \( \mathbf{b}[k] \) is defined as follows:

\[ \mathbf{b}[k] = \begin{bmatrix} b_1[k] \\ b_2[k] \end{bmatrix} \]
The values for $b[k]$ can be optimized by the linear least square method:

$$b[k] = \left( X'[k]X[k] \right)^{-1} X'[k]y[k]$$  \hfill [41]

In this work, we use the recursive least square (RLS) procedure\textsuperscript{15} to estimate $b[I]$ values at each time instance to reduce the memory requirement, and the details for this method are presented in Appendix B. With the optimized $b_1[k]$ and $b_2[k]$ values, the $V_j$ value in the ROM Eq. 4 can be estimated at current $I' = I + \Delta I$ by the following state space equation:

$$V'_j[k] = b_1[k]V'_0[k - 1] + b_2[k]I'[k - 1]$$  \hfill [43]

and $V'_0[k]$ is calculated by:

$$V'_0[k] = \bar{V}_d[k] + V_0[k]$$  \hfill [44]

The advantage of using Eq. 43 and 44 instead of Equation 42 to estimate $V'_0$ is explained as follows: in Equation 43, the errors in the optimized parameters $b_1[k]$ and $b_2[k]$ are scaled by $V'_0[k - 1]$ and $I'[k - 1] - I[k - 1]$; in Equation 42, however, these errors are scaled respectively by $V'_0[k - 1]$ and $I'[k - 1]$; as the magnitudes $|I'[k - 1] - I[k - 1]| < |I'[k - 1]|$ and $|V'_0[k - 1]| < |V'_0[k - 1]|$, Equation 43 would generate less error than Equation 42.

**Battery module implementation.**—In this work, the ROM algorithm was implemented on a battery module as illustrated in Figure 1. This battery module includes 24 cells connected in parallel (24P module) by two busbars, and the positive and negative electrodes of each cell are welded to busbars through tabs. The cells in this battery module are labeled as cell #01 through cell #24, $I_i$ and $V_j$ (i = 1, 2, ···, 24) respectively stand for current and voltage of each cell, $\Phi_{p,i}$ and $\Phi_{n,i}$ respectively stand for the positive and negative busbar potentials of each cell, $\Phi_{T,p}$ and $\Phi_{T,n}$ are respectively positive and negative busbar potentials at the external battery terminals, $R_{\text{Busbar}}$ is the busbar resistance between two adjacent cells, $R_{\text{Tab}}$ is the tab resistance of each cell, and $I_T$ is the total current passing through module. All the cells are assumed to have identical design and properties, and thermal effects are neglected. According to Figures 1b and 1c, the following equations can be derived for the busbar potentials:

$$\frac{\Phi_{p,i} - \Phi_{p,i+1}}{R_{\text{Busbar}}} = - \sum_{j=1}^{i} I_j \frac{\Phi_{n,j} - \Phi_{n,j+1}}{R_{\text{Busbar}}} = \sum_{j=1}^{i} I_j \ (i = 1, 2, \cdots 11)$$  \hfill [45]

$$\frac{\Phi_{p,i} - \Phi_{T,p}}{R_{\text{Busbar}}} = - \sum_{j=1}^{10} I_j \frac{\Phi_{n,j} - \Phi_{T,n}}{R_{\text{Busbar}}} = \sum_{j=1}^{10} I_j \ (i = 12)$$  \hfill [46]

$$\frac{\Phi_{p,i} - \Phi_{T,p}}{R_{\text{Busbar}}} = - \sum_{j=1}^{24} I_j \frac{\Phi_{n,j} - \Phi_{T,n}}{R_{\text{Busbar}}} = \sum_{j=1}^{24} I_j \ (i = 13)$$  \hfill [47]
Figure 2. Flowchart for multi-cells simulation (a) the full-order P2D model block, (b) estimation of ROM parameters, (c) the ROM block.

The overall current balance for the module is described as follows:

\[ I_T = \sum_{j=14}^{24} I_j \]  \[(49)\]

and the terminal of negative busbar is chosen for potential reference

\[ \Phi_{T,n} = 0 \] \[(50)\]

For each cell, the correlation between busbar potentials and cell voltages are given by:

\[ \Phi_{p,i} - \Phi_{n,i} = V_i + I_i R_{Busbar} \quad (i = 1, 2, \ldots, 24) \] \[(51)\]

To estimate cell voltage \( V_i \), a straightforward method is to apply full-order P2D model to each cell. The flowchart for a P2D model block is illustrated by Figure 2a: at time instance \( t[k] \), the cell current
I[k] goes through a computational block which contains all P2D model equations and returns the instantaneous voltage response $V_{i[k]}$ which equals to $V_{P2D,i}$. An alternative approach is to replace the P2D models by the ROM, but before implementing ROM for each cell, certain parameters need to be evaluated first. As shown in Figure 2b, the terminal current $I_{T}[k]$ divided by the total cell number to yield the average cell current $\bar{I}[k]$, then the signal $\bar{I}[k]$ enters a stand-alone P2D block to return several variables: $\delta_{V}[k]$, $u_{V}[k]$, $J_{e}[k]$, $J_{l}[k]$, and $\delta_{b}[k]$ : based on these outputs from the P2D block, values for certain ROM variables $V_{i[k]}$, $V_{d[k]}$, and $R_{l}[k]$ can be calculated; in addition, variable $V_{d}[k]$ is fed into a recursive least square (RLS) filter to estimate the diffusion parameters $b[k]$. According to Figure 2c, with the optimized parameters ($V_{i[k]}$, $V_{d[k]}$, $R_{l}[k]$, and $b[k]$), the ROM can be applied to estimate the voltage of individual cells under different current inputs; in this case, $V_{i[k]}$ equals the ROM voltage $V_{ROM,i}$.

### Results and Discussion

According to the discussion above, the 24P battery model can be solved by either running 24 full-order P2D models (FOM method) or using 24 ROMs with a stand-alone P2D model (ROM method). Comprising only two state variable equations and a few explicit algebraic expressions, the ROM significantly reduces the complexity of a P2D model which involves several non-linear PDEs. To verify the strength of our approach, both FOM and ROM methods were first implemented to simulate an aggressive drive cycle. The parameter values for battery cells are given in Table I and the input current profile for the drive cycle is presented in Figure 3. The peak discharge current for the drive cycle is equivalent to 2.0C (12A in average for all the cells) and the sampling frequency is 1 Hz. This simulation was performed by MATLAB/Simulink software, the computation time for FOM is 104.8 sec and for ROM is 1.95 sec. Figure 4 shows the simulated voltage results by FOM and ROM, where the voltage profiles of battery terminals and three cells (#01, #12, and #18) are compared. Zoom-up plots are presented in each case to catch the details of voltage comparisons. The root-square-mean-deviations (RMSD) between FOM and ROM are calculated for each plot in Figure 4. The simulated FOM and ROM current profiles for cell #01, #12, and #18 are shown in Figure 5 with zoom-up plots and calculated RMSD. The simulation results in Figure 4 and Figure 5 suggest that the ROM achieves about 97% accuracy.

### Table I. Parameters for the pseudo-2D model.

| Parameter | Anode | Separator | Cathode |
|-----------|-------|-----------|---------|
| Thickness $l_{a}$, $l_{s}$, $l_{p}$ [m] | 70 × 10⁻⁶ | 25 × 10⁻⁶ | 50 × 10⁻⁶ |
| Volume fraction of electrolyte $\epsilon_{e}$ | 0.4 | 0.4 | 0.4 |
| Volume fraction of active material $\epsilon_{a}$ | 0.51 | 0.41 | 0.41 |
| Specific surface area $\alpha$ [1/m] | 3.01 × 10⁶ | 7.5 × 10⁴ | 7.5 × 10⁴ |
| Maximum Li concentration in solid phase $c_{max}$ [mol/m³] | 2.87 × 10⁶ | 4.9 × 10⁴ | 4.9 × 10⁴ |
| Electrical conductivity of solid phase $\sigma_{s}$ [S/m] | 100 | 3.8 | 3.8 |
| Diffusivity of solid phase $D_{s}$ [m²/s] | 9 × 10⁻¹⁴ | 3 × 10⁻¹⁵ | 3 × 10⁻¹⁵ |
| Reference state exchange current density $j_{es}$ [A/m²] | 74.56 | 8.13 | 8.13 |
| Film resistance $R_{film}$ [$\Omega \cdot m²$] | 0.71 | 0.015 | 0.015 |
| Bulk electrolyte diffusivity $D_{bulk}$ [m²/s] | 1.1 × 10⁻¹⁰ | 0.363 | 0.363 |
| Transference number of electrolyte $\lambda$ | 0.3325 | 1200 | 1200 |
| Area of the cathode/current collector interface $A_{c}$ [m²] | 96487 | 8.3143 | 8.3143 |
| Average electrolyte concentration $c_{e}$ [mol/m³] | 70 | 25 | 25 |
| Universal gas constant $R$ [J/mol/K] | 14 3 | 0.363 | 0.363 |
| Faraday constant $F$ [C/mol] | 14 3 | 0.363 | 0.363 |
| Temperature $T$ [°C] | 207.24 | 8.13 | 8.13 |
| Busbar resistance $R_{busbar}$ [$\Omega$] | 96487 | 8.3143 | 8.3143 |
| Tab resistance $R_{tab}$ [$\Omega$] | 20.0 A | 10 × 10⁻⁴ | 10 × 10⁻⁴ |

In Figures 7a through 7e, the key ROM parameters ($R_{c}[k]$, $V_{i}[k]$, $V_{d}[k]$, and $b[k]$) are plotted versus depth-of-discharge for the drive cycle and CC discharge cases. The electrical resistance ($R_{c}[k]$) and electrical over-voltage ($V_{d}[k]$) are derived from the nonlinear Butler-Volmer equations, therefore these two parameters are dependent on the instantaneous current inputs. Consequently, values for $R_{c}[k]$ and $V_{d}[k]$ change rapidly during the high-frequency drive cycle but take smooth profiles under constant currents. For diffusional over-voltage $V_{d}[k]$, as there is a time delay in its response, the $V_{d}[k]$ values oscillate around a negative offset during the drive cycle. According to the 0.5C curve in Figure 7c, $V_{d}[k]$ drops significantly when DOD exceeds 90%, which is caused by the depletion of intercalation sites at the surface of cell #12; these values deviate from the average current by 70%, so the ROM has good confidence to predict the electrical imbalances in a battery. Besides the high-frequency drive cycle, FOM and ROM are also used to simulate constant current (CC) discharges with 0.5C, 1C, and 2C. The profiles for terminal voltage vs depth-of-discharge (DOD) for different CC cases are displayed in Figure 6, and the computation time and RSMD values for each case are listed in Table II. The above simulation results show that ROM is 50–70 times faster than FOM. However, note that in our simulation, the FOM has already been sped up by the NSVM method (50–100 times faster than COMSOL solver according to References 8 and 9), therefore the time-efficiency of ROM is significant. Although its accuracy decreases with current magnitude, the ROM method still exhibits outstanding performance considering the low computational cost.

Figure 3. Current profile for a practical drive cycle.
Figure 4. Comparisons of voltage results between FOM and ROM, (a) the terminal voltage defined as $\Phi_{T,p} - \Phi_{T,n}$, (b) the voltage for cell#01, (c) the voltage for cell#12, (d) the voltage for cell#18.
Figure 5. Comparisons of current results between FOM and ROM (a) cell #01, (b) cell #12, (c) cell #18.
cathode. The two diffusional parameters $b_1[k]$ and $b_2[k]$ take smooth profiles during all four cases except for a short unstable initial period. The reason is that $b_1[k]$ and $b_2[k]$ are estimated recursively from initial guesses, and it may take several iterations to settle these parameter values. As shown in Figure 7, the profiles for a specific parameter vary dramatically in different operation cases. These results suggest that our ROM is an adaptive algorithm, which means the parameter values can be optimized according to the real-time current inputs; if the input signal changes, the algorithm is able to re-evaluate parameters to achieve higher accuracy.

Table II. Computation time and RSMD for 0.5C, 1C, and 2C discharges.

| Computation time (sec) | Computation time (sec) | Computation time (sec) |
|------------------------|------------------------|------------------------|
| 0.5C                   | 140.2                  | 2.63                   | 0.0058                  |
| 1C                     | 155.5                  | 2.30                   | 0.0073                  |
| 2C                     | 73.5                   | 1.39                   | 0.0089                  |

**Figure 6.** Simulated voltage profiles for 0.5C, 1C, and 2C discharges.

**Figure 7.** Plots of ROM parameters vs DOD for different cases: (a) electrical resistance, (b) electrical over-voltage, (c) diffusional over-voltage, (d) parameter $b_1$, (e) parameter $b_2$. 
Conclusions and Future Work

A reduced-order-modeling (ROM) method was developed for the P2D Li-ion cell model based on the specific solution procedure of the NSVM algorithm. By sharing the real-time parameters estimated by a stand-alone P2D model, the ROM, which shows great accuracy and adaptiveness for various operation conditions, can be distributed into different cells in a battery pack. Compared with the full-order-model (FOM), which employs distributed P2D models and is solved by the NSVM, the ROM improves the computation efficiency by 50–70 times. The ROM only contains two state equations (one for \( \theta_n[k] \) and the other one for \( V_{udk}[k] \)), and its numerical complexity is just comparable to a 1-RC equivalent circuit model. As a stand-alone P2D model is a pre-request for running the ROM, only when used for simulating large battery systems can the advantages of ROM be realized.

In the future, this ROM approach can potentially be used to couple with heat transfer equations in the Multi-Scale-Multi-Dimensional (MSMD) framework,\(^\text{16}\) and model the distributed electrical and thermal behavior inside the cell volume. The feasibility for this proposed transformation is based on the model structure in Reference 17, where the planar electrode pair is treated as a 2D circuit network, and the ROM would replace the electrochemical model to compute the current flow at each grid.

Appendix A

Illustrations of the porous electrode domains for the P2D model are shown in Figure A1 and the governing equations are summarized in Table A1. The open circuit potential expressions are given below:

\[
U_o = 0.124 + 1.5 \exp(-700 - 0.0355 \text{tanh}(12.04829 - 3.4458))
- 0.0045 \text{tanh}(8.4034 - 7.5630) - 0.035 \text{tanh}(2000 - 19.80)
- 0.0147 \text{tanh}(29.41180 - 14.7059) - 0.102 \text{tanh}(7.04239 - 1.3662)\ [A1]
- 0.022 \text{tanh}(60.97569 - 59.7561) - 0.011 \text{tanh}(44.24780 - 5.4867)
- 0.0155 \text{tanh}(34.48280 - 3.6207)
\]

Table A1. Governing equations for the P2D model.

| Physics                          | Equations |
|----------------------------------|-----------|
| Electrolyte diffusion            | \[
\frac{\partial \eta_{\text{L}}}{\partial t} = \frac{e}{\varphi_{\text{L}}} \left( D_{\text{eff}} \frac{\partial \eta_{\text{L}}}{\partial x} + a(1 - r^t) \frac{\partial \eta}{\partial \Phi} \right) + \frac{e}{\varphi_{\text{L}}} \left( \eta_{\text{L}} ^{\text{eff}} \frac{\partial \eta_{\text{L}}}{\partial x} + \eta_{\text{L}} \right)
\]

(Defined through \( 0 \leq x \leq l_n + l_b + l_p \) where \( j_{\text{L}} = 0 \) for \( l_n \leq x \leq l_n + l_b \)) |
| Electrolyte charge conservation  | \[
\frac{\partial \eta}{\partial t} = \frac{e}{\varphi_{\text{L}}} \left( k_{\text{eff}} 2RT \left( \frac{\partial \eta}{\partial \Phi} + \frac{\partial \eta_{\text{L}}}{\partial \Phi} \right) + a j_{\text{L}} \right)
\]

(Defined through \( 0 \leq x \leq l_n + l_b + l_p \) where \( j_{\text{L}} = 0 \) for \( l_n \leq x \leq l_n + l_b \)) |
| Solid phase charge conservation  | \[
\frac{\partial \sigma_{\text{S}}}{\partial t} = -i_{\text{in}}(t) \quad \frac{\partial \sigma_{\text{S}}}{\partial x} |_{x=0} = 0 \quad \frac{\partial \sigma_{\text{S}}}{\partial x} |_{x=l_n+l_b+l_p} = 0 \quad \frac{\partial \sigma_{\text{S}}}{\partial x} |_{x=l_n+\text{L}_{\text{eff}}} = \frac{\partial \sigma_{\text{S}}}{\partial x} |_{x=\text{L}_{\text{max}}} = 0
\]

(Defined only for \( 0 \leq x \leq l_n \) and \( l_n + l_b \leq x \leq l_n + l_b + l_p \)) |
| Solid phase diffusion            | \[
\frac{\partial \eta}{\partial t} = \frac{D_S}{\eta} \left( \frac{\partial}{\partial x} \left( \frac{\sigma_{\text{S}}}{\eta} \right) \right) \quad \frac{\partial \sigma_{\text{S}}}{\partial x} |_{x=0} = 0 - \frac{D_S}{\eta} \frac{\partial \sigma_{\text{S}}}{\partial x} |_{x=RT} = \frac{\partial \sigma_{\text{S}}}{\partial x} |_{x=R_{\text{max}}} = 0
\]

(Defined only for \( 0 \leq x \leq l_n \) and \( l_n + l_b \leq x \leq l_n + l_b + l_p \)) |
| Butler-Volmer equation          | \[
\eta = \phi_{\text{s}} - \phi_{\text{L}} - j_{\text{s}} R_{\text{lim}} - U
\]

\( j_{\text{s}} = j_{\text{ca}} (1 - \theta)^{0.5} \left( \frac{l_n}{c_{\text{f}}} \right)^{0.5} \left( \frac{c_{\text{f}}}{l_n} \right)^{0.5} [\exp(0.5 \frac{\Phi}{RT}) - \exp(-0.5 \frac{\Phi}{RT})]
\]

(Defined only for \( 0 \leq x \leq l_n \) and \( l_n + l_b \leq x \leq l_n + l_b + l_p \)) |
| External conditions             | \[
I = -i_{\text{in}}(t) A_{\text{C}}
\]
And $\mathbf{X}[k]\mathbf{N}[k]$ and $\mathbf{X}[k]\mathbf{1}[k]$ can be respectively expressed by:

$$\mathbf{X}[k]\mathbf{N}[k] = \sum_{j=0}^{k} \mathbf{1}[j]\mathbf{1}[k] \quad \mathbf{X}[k]\mathbf{1}[k] = \sum_{j=0}^{k} \mathbf{1}[j]y[j] \quad [B3]$$

The following equations can be derived according to Equation B3:

$$\mathbf{X}'[k-1]\mathbf{N}[k-1] = \sum_{j=0}^{k-1} \mathbf{1}[j]\mathbf{1}[k-1] = \mathbf{X}[k]\mathbf{N}[k] - \mathbf{X}[k-1]\mathbf{1}[k] \quad \mathbf{X}'[k-1]y[k-1] = \sum_{j=0}^{k-1} \mathbf{1}[j]y[k] = \mathbf{X}[k]\mathbf{1}[k] - \mathbf{X}[k-1]y[k] \quad [B4]$$

where $\mathbf{1}[j]$ is the $j$th row vector of the matrix $\mathbf{1}$. Substitute Equation B4 into B2 to yield

$$\left(\mathbf{X}[k]\mathbf{N}[k] - \mathbf{X}[k-1]\mathbf{1}[k]\right)\mathbf{h}[k] = \mathbf{X}[k]\mathbf{1}[k]y[k]$$

$$\mathbf{X}[k]\mathbf{N}[k] - \mathbf{X}[k-1]\mathbf{1}[k] = \mathbf{X}[k]\mathbf{1}[k]y[k] \quad [B5]$$

and the following equation can be derived by subtracting Equation B5 from Equation B1:

$$\mathbf{X}[k]\mathbf{N}[k] - \mathbf{X}[k-1]\mathbf{1}[k] = \mathbf{X}[k]\mathbf{1}[k]y[k] - \mathbf{X}[k]y[k] = \mathbf{X}[k]\mathbf{1}[k][B6]$$

Left multiply Equation B6 by $\mathbf{X}'[k]\mathbf{N}[k][B1]$ and rearrange terms to get the following recursive expression for $\mathbf{h}[k]$:

$$\mathbf{h}[k] = \mathbf{h}[k-1] + \left(\mathbf{X}'[k]\mathbf{N}[k]\right)^{-1} \mathbf{X}'[k]y[k]$$

Instead of recording all history, the value for $\mathbf{X}[k]\mathbf{N}[k]$ can be updated at each time instance using:

$$\mathbf{X}[k]\mathbf{N}[k] = \mathbf{X}[k-1]\mathbf{1}[k-1] + \mathbf{X}[k]y[k] \quad [B8]$$

In our specific case, $\mathbf{X}[k]\mathbf{N}[k]$ is a 2 x 2 symmetric matrix which can be expressed as follows:

$$\mathbf{X}[k]\mathbf{N}[k] = \begin{bmatrix} f[k] & g[k] \\ g[k] & h[k] \end{bmatrix} \quad [B9]$$

and the elements $f[k], g[k],$ and $h[k]$ are estimated by:

$$f[k] = f[k-1] + \chi_1[k]\chi_2[k] \quad g[k] = g[k-1] + \chi_1[k]\chi_2[k] \quad h[k] = h[k-1] + \chi_2[k] \quad [B10]$$

where $\chi_1[k]$ and $\chi_2[k]$ are respectively the 1st and 2nd element of vector $\mathbf{X}[k]$. Therefore, the covariance matrix is estimated as follows:

$$\left(\mathbf{X}'[k]\mathbf{N}[k]\right)^{-1} = \frac{1}{f[k]h[k] - g^2[k]} \begin{bmatrix} h[k] & -g[k] \\ -g[k] & f[k] \end{bmatrix} \quad [B11]$$

Substitute Equations B11 into B7, and the individual parameters $b_1[k]$ and $b_2[k]$ can be calculated using the following equations:

$$b_1[k] = b_1[k-1] + K_{RLS}\chi_1[k] \quad b_2[k] = b_2[k-1] + K_{RLS}f[k] \chi_2[k] \quad [B12]$$

where the expression for the gain value $K_{RLS}$ is given by:

$$K_{RLS} = \frac{\gamma[k] - b_1[k-1] \chi_1[k] + b_2[k-1] \chi_2[k]}{f[k]h[k] - g^2[k]} \quad [B13]$$

### List of Symbols

| Symbol | Description | Unit | Source |
|--------|-------------|------|--------|
| $a$    | Solid phase specific surface area in general form | m² |        |
| $a_{s,n}$ | Solid phase specific surface area for anode | m² |        |
| $a_{s,p}$ | Solid phase specific surface area for cathode | m² |        |
| $A_c$  | Coating area of cathode | m² |        |
| $B$    | Parameter vector for RLS | m² |        |
| $b$    | Parameter for diffusion voltage | V |        |
| $b_1$  | Parameter for diffusion voltage | V |        |
| $c_0$  | Reference concentration of electrolyte | mol/m³ |        |
| $c_L$  | Concentration of electrolyte | mol/m³ |        |
| $c_S$  | Concentration of Li in solid phase | mol/m³ |        |
| $c_{s,max}$ | Maximum Li concentration of solid phase in general form | mol/m³ |        |
| $c_{s,n,max}$ | Maximum Li concentration of solid phase | mol/m³ |        |
| $c_{s,p,max}$ | Maximum Li concentration of solid phase in cathode | mol/m³ |        |
| $C_0$  | Integral constant | mol/m³ |        |
| $d$    | Source term vector | m³/s |        |
| $D_{L,bulk}$ | Diffusivity of bulk electrolyte | m²/s |        |
| $D_0$  | Effective diffusivity of electrolyte in porous media | m²/s |        |
| $F$    | Faraday constant | C/mol |        |
| $f_B$  | Inward current density at cathode/foil boundary | A/m² |        |
| $I$    | Current on P2D model | A |        |
| $I_A$  | Average current of battery | A |        |
| $I_E$  | Current of each cell in a battery | A |        |
| $I_T$  | Current on battery terminal | A |        |
| $J$    | Remaining part of Jacobian matrix | J/mol/(s·m²) |        |
| $J_d$  | Right-most column of Jacobian matrix | J/mol/(s·m²) |        |
| $J_{Busbar}$ | Resistance of busbar | Ω |        |
| $R$    | Resistance of surface film | Ω |        |
| $R_{Gab}$ | Resistance of GB | Ω |        |
| $R_{N}$ | General format for the radius of solid particle | m |        |
| $R_{N,a}$ | Radius of anode solid particle | m |        |
| $R_{N,p}$ | Radius of cathode solid particle | m |        |
| $R_{Tab}$ | Resistance of Tab | Ω |        |
| $t$    | Time | s |        |
| $T$    | Temperature | K |        |
| $u_{I_B}$ | Long-time variable for linear voltage expression | V |        |
| $U$    | Open circuit potential in general format | V |        |
| $U_{eq}$ | Equilibrium open circuit voltage of P2D model | V |        |
| $U'_{eq}$ | Equilibrium open circuit voltage of ROM | V |        |
| $U_{eq}$ | Open circuit potential of anode | V |        |
| $U_{eq,c}$ | Open circuit potential of cathode | V |        |
| $\phi_{0}$ | Diffusional over voltage of P2D model | V |        |
| $\phi_{0,c}$ | Diffusional over voltage of ROM | V |        |
| $\phi_{0}$ | Difference in diffusional voltage between P2D and ROM | V |        |
| $\phi_{0,c}$ | Electrical over-voltage of P2D model | V |        |
| $\phi_{0,c}$ | Electrical over-voltage of ROM | V |        |
| $\phi_{0,c}$ | Voltage of each cell in a battery | V |        |
| $\phi_{0,c}$ | Cell voltage computed by P2D model | V |        |
| $\phi_{0,c}$ | Cell voltage computed by ROM | V |        |
| $\chi$ | Linear coordinate | m |        |
| $\chi_{2}$ | Vector for discretized concentrations | mol/m³ |        |
| $\chi_{2,n}$ | Independent variable matrix for RLS | mol/m³ |        |
| $\chi_{2,n}$ | Dependent variable vector for RLS | mol/m³ |        |
| $\chi_{2,p}$ | Instantaneous resistance for linear voltage expression | Ω·m² |        |

**Greek**

| Symbol | Description | Unit | Source |
|--------|-------------|------|--------|
| $\alpha$ | Porosity of media | | |
Φ

n,i

Negative busbar potential for each cell in battery V
Φ

p,i

Positive busbar potential for each cell in battery V
Φ

T,n

Potential of negative battery terminal V
Φ

T,p

Potential of positive battery terminal V
η

Electrode over potential V
κ

L,bulk

Electrical conductivity of bulk electrolyte S/m
κ

L

Effective conductivity of electrolyte S/m
A

A

Matrix operator for NSVM state equation
\frac{\partial}{\partial t}

Dimensionless concentration at the surface of particle
θ

avg

Dimensionless particle-average concentration of Li
θ

n

Dimensionless anode-average concentration of Li
θ

p

Dimensionless cathode-average concentration of Li
σ

S

Effective conductivity of solid phase
σ

S

Effective conductivity of solid phase
τ

d

Time constant for diffusional over-voltage s

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