Diff and Merge

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Abstract

Accurate estimation of dynamic direct current internal resistance (DCIR) in lithium-ion cells remains one of the most critical, yet unresolved, modeling bottlenecks in industrial Battery Management Systems (BMS). Conventional voltage-drop based DCIR estimation — while computationally attractive — collapses under non–steady-state excitation, state-of-charge (SOC) dependent hysteresis, temperature-dependent transport losses, and slow relaxation modes that manifest in multi-time-constant impedance behavior. This paper introduces a **physics-informed hybrid modeling framework** that unifies:
(1) a 2-RC Equivalent Circuit Model (ECM) as a physically interpretable dynamic prior,
(2) a differentiable Runge–Kutta solver (Neural ODE) to propagate continuous-time electrochemical state trajectories, and
(3) a temperature-aware residual neural network that learns structured unmodeled dynamics (aging, hysteresis, SEI-layer drift, localized diffusion losses).

Unlike conventional ML regressors, the neural component is never tasked with learning the forward dynamics "from scratch"; instead it learns only the error manifold **orthogonal to physics**, dramatically improving generalization and identifiability.
We further introduce a Bayesian Kalman filtering layer for online inference — allowing parametric DCIR to be tracked in real-time under arbitrary excitation waveforms. Synthetic campaigns and preliminary real-cell validations demonstrate that the hybrid architecture consistently outperforms voltage-drop approaches and pure RK-ECM simulation, particularly in regimes with sharp current steps, high dI/dt, thermal gradients, and low-SOC driving conditions. This establishes a generalizable methodology for cell-level DCIR estimation that scales to real pack operation and aligns directly with the future direction of industrial predictive battery control.

Nomenclature

$\mathbf{v_{c1}}, \mathbf{v_{c2}}$ Voltage across first and second RC polarization branches (V)
SOC State of Charge (–)
T Cell temperature (°C or K)
$\mathbf{I(t)}$ Applied current (positive = discharge) (A)
$\mathbf{V(t)}$ Terminal cell voltage (V)
$\mathbf{OCV(SOC, T)}$ Open-circuit voltage as function of SOC & temperature (V)

$\mathbf{R_0}$	Instantaneous ohmic resistance (Ω)
$\mathbf{R_1}, \mathbf{R_2}$	Polarization resistances (slow & fast modes) (Ω)
$\mathbf{C_1}, \mathbf{C_2}$	Polarization capacitances (slow & fast modes) (F)
$\mathbf{Q}$	Nominal cell capacity (As or Ah)
η	Coulombic efficiency (–)
$\dot{\mathbf{x}}$	Time derivative of state vector ((various))
$\hat{\mathbf{V}}$	Model-predicted voltage (V)
$\mathbf{\Delta V}_\theta$	Neural-network residual correction (V)
$\mathbf{L}(\theta)$	Training loss (voltage domain) (V^2)
$\mathbf{F_{RK4}}(\cdot)$	Runge-Kutta 4th-order time propagator (–)
KF	Kalman Filter (–)
DCIR	Direct Current Internal Resistance (Ω)

1 Introduction

[*** — ***]

Reliable estimation of a lithium-ion cell's **DC internal resistance (DCIR)** under real operating conditions is central to modern battery management systems (BMS). DCIR governs instantaneous **power capability**, **heat generation**, and **voltage sag**, thereby affecting **driver-perceived performance** (acceleration, regen), **safety margins** (thermal run-away risk), and **state-of-health** (SOH) diagnostics. In electric vehicles and stationary storage, the estimator must remain **accurate across a wide range of currents**, **temperatures, and states of charge (SOC)**; it must be **computationally light**, **data-efficient**, and **stable** under measurement noise. Meeting all of these simultaneously is difficult because the cell's terminal behavior couples fast interfacial phenomena (double-layer charging, SEI, contact resistances) and slow diffusion/transport effects (porous electrode and electrolyte transport), each with different time scales and temperature sensitivities. Any estimator that collapses this multiscale structure into a single lumped constant tends to be biased, especially during transients—which is precisely when the BMS needs accurate predictions.

[... Intro ...]

2 Literature Review / Related Work

[... ...]

3 Methodology

This section presents the proposed hybrid DCIR estimation framework in full detail. The model is built around a temperature-aware, two-branch equivalent circuit representation (2RC ECM) embedded in a differentiable ODE integrator (RK4), with two neural submodules: a parameter head that maps operating conditions to physically constrained ECM parameters, and a residual head that corrects remaining voltage mismatch stemming from hysteresis, aging, or unmodeled pack effects. The overall design preserves physical interpretability, supports end-to-end learning from raw current–voltage–temperature

sequences, and yields a DCIR read-out that is both transient-aware and aligned with industrial Voltage-Drop practices.

3.1 Overall formulation and problem statement

[... ...]

3.2 Two-RC equivalent circuit model (state-space form)

[... 2RC ECM ( ) ...]

We model two polarization branches and the bulk charge inventory:

$$x = \begin{bmatrix} v_{c1} \\ v_{c2} \\ SOC \end{bmatrix}, \qquad V = OCV(SOC) - R_0 I - v_{c1} - v_{c2} + \Delta V_\phi.$$

The continuous-time dynamics are:

$$\dot{v}_{c1} = -\frac{v_{c1}}{R_1 C_1} + \frac{I}{C_1}, \qquad \dot{v}_{c2} = -\frac{v_{c2}}{R_2 C_2} + \frac{I}{C_2}, \qquad \dot{SOC} = \frac{\eta}{Q} I.$$

[... ...]

3.3 Classical 1RC ECM DCIR Baseline (for Comparison)

For completeness and for comparison to existing practice, we also implement a **classical single-RC (1RC) Thevenin model** with a multiplicative parametric law for the ohmic resistance $R_0(T, SOC, SOH, C_r)$. This baseline is *not* our final proposal, but serves as a reference against which the benefits of the 2RC Neural ODE framework can be quantified.

The 1RC ECM uses the states

$$x_{\text{1RC}} = \begin{bmatrix} v_{RC} \\ SOC \end{bmatrix},$$

with terminal voltage

$$V_{\text{model}}(t) = OCV(SOC(t), T(t)) - R_0(T, SOC, SOH, C_r)\, I(t) - v_{RC}(t). \tag{1}$$

The polarization branch follows

$$\frac{dv_{RC}}{dt} = -\frac{1}{R_1 C_1} v_{RC} + \frac{1}{C_1} I(t), \tag{2}$$

and the SOC evolves according to Coulomb counting

$$\frac{dSOC}{dt} = -\frac{I(t)}{Q_{\text{nom}}}, \tag{3}$$

with nominal capacity Q_{nom}.

The ohmic resistance R_0 is expressed as a product of scalar correction factors:

$$R_0(T, SOC, SOH, C_r) = R_{0,\text{ref}}\, F_T(T; E_a)\, F_{SOC}(SOC; \beta)\, F_{SOH}(SOH; \gamma)\, F_C(C_r; \kappa), \tag{4}$$

where $R_{0,\mathrm{ref}}$ is a reference resistance at nominal conditions and $F_T, F_{SOC}, F_{SOH}, F_C$ are empirical temperature, SOC, aging, and C-rate factors, respectively. Their detailed forms and Jacobians are summarized in Appendix A.

This 1RC baseline is identified with a Gauss–Newton / Levenberg–Marquardt optimizer acting on (4) under fixed R_1, C_1, and is used only as:

- a conventional ECM-style DCIR estimator for comparison with $\hat{R}_0(SOC, T)$ from our Neural ODE,
- an ablation point illustrating the structural limitations of 1RC (single time constant) versus the proposed 2RC backbone.

3.4 Temperature-aware parameterization (neural parameter head

[... , "ealized" → "realized" ...]

3.5 Residual voltage correction (neural residual head)

[... ...]

3.6 Differentiable RK4 integration

We integrate continuous dynamics using the classical **Runge–Kutta 4th order** at the BMS sampling rate. Let $f(x, I, \theta_{p,k})$ denote the right-hand side where $\theta_{p,k} = (R_{1,k}, C_{1,k}, R_{2,k}, C_{2,k}, Q, \eta)$. For step k:

$$k_1 = f(x_k, I_k; \theta_{p,k}), \tag{5}$$
$$k_2 = f\big(x_k + \tfrac{\Delta t}{2} k_1, I_k; \theta_{p,k}\big), \tag{6}$$
$$k_3 = f\big(x_k + \tfrac{\Delta t}{2} k_2, I_k; \theta_{p,k}\big), \tag{7}$$
$$k_4 = f(x_k + \Delta t\, k_3, I_k; \theta_{p,k}), \tag{8}$$
$$x_{k+1} = x_k + \frac{\Delta t}{6}\big(k_1 + 2k_2 + 2k_3 + k_4\big). \tag{9}$$

[... : Loss, OCV modeling, sign conventions, identifiability, pseudocode ...]

4 Data, Preprocessing, and Sign Conventions

[... ...]

5 Experiment Protocol

[... , Baseline "1RC ECM + parametric R_0 (Appendix A)" ...]
: Baseline :
We compare against:

- classical Voltage-Drop DCIR R_{drop},
- a 1RC ECM with parametric $R_0(T, SOC, SOH, C_r)$ identified via Gauss–Newton / LM (Appendix A),

- 2RC ECM without residuals,
- purely data-driven ML regressors (where appropriate).

6 Experiments

[... "expected results" , / ...]

7 Discussion

[... ...]

8 Conclusion

[... ...]

A Classical 1RC ECM DCIR Estimator (Baseline)

This appendix summarizes the traditional 1RC ECM-based DCIR estimator that we implement as a baseline. It closely follows the standard Thevenin model with a single RC branch and an empirical multiplicative law for $R_0(T, SOC, SOH, C_r)$.

A.1 1RC Equivalent Circuit Model

The Thevenin 1RC model consists of:

- an ohmic resistance R_0,
- a polarization branch with resistance R_1 and capacitance C_1 in parallel,
- a nonlinear open-circuit voltage source $OCV(SOC, T)$.

With discharge-positive current $I(t)$, the modeled terminal voltage is

$$V_{\text{model}}(t) = OCV(SOC(t), T(t)) - R_0(T, SOC, SOH, C_r)\, I(t) - v_{RC}(t), \tag{10}$$

where $v_{RC}(t)$ is the voltage across the R_1–C_1 branch.

The polarization dynamics obey

$$\frac{dv_{RC}}{dt} = -\frac{1}{R_1 C_1} v_{RC}(t) + \frac{1}{C_1} I(t), \tag{11}$$

and the SOC follows Coulomb counting:

$$\frac{dSOC}{dt} = -\frac{I(t)}{Q_{\text{nom}}}. \tag{12}$$

In our baseline, R_1 and C_1 are treated as constants calibrated from laboratory pulses; the focus is on identifying the structured dependence of R_0 on operating conditions.

A.2 Multiplicative Parameterization of R_0

We adopt the multiplicative form

$$R_0(T, SOC, SOH, C_r) = R_{0,\text{ref}}\, F_T(T; E_a)\, F_{SOC}(SOC; \beta)\, F_{SOH}(SOH; \gamma)\, F_C(C_r; \kappa), \quad (13)$$

where:

- $R_{0,\text{ref}}$ is a reference resistance at nominal conditions,
- F_T is a temperature factor (Arrhenius-type),
- F_{SOC} describes SOC dependence,
- F_{SOH} (or F_{age}) accounts for aging,
- F_C encodes C-rate dependence.

(a) Temperature dependence.

$$F_T(T; E_a) = \exp\left[\frac{E_a}{R_g}\left(\frac{1}{T} - \frac{1}{T_{\text{ref}}}\right)\right], \quad (14)$$

where E_a is an activation energy and $R_g \approx 8.314\,\text{J}\,\text{mol}^{-1}\,\text{K}^{-1}$ is the universal gas constant.

(b) SOC dependence. We use a quadratic correction:

$$F_{SOC}(SOC; \beta_1, \beta_2) = 1 + \beta_1(1 - SOC)^2 + \beta_2(SOC)^2, \quad (15)$$

capturing resistance rise at low and high SOC due to overpotential effects.

(c) Aging dependence. Two equivalent forms are commonly used:

$$F_{SOH}(SOH; \gamma_1) = 1 + \gamma_1(1 - SOH), \quad (16)$$

or, as a function of aging time t_{age},

$$F_{\text{age}}(t_{\text{age}}; k_{\text{age}}) = 1 + k_{\text{age}}\sqrt{t_{\text{age}}}. \quad (17)$$

(d) C-rate dependence. Rate effects are modeled as

$$F_C(C_r; \kappa_1, \kappa_2) = 1 + \kappa_1|C_r|^{\kappa_2}, \quad (18)$$

with C_r the instantaneous C-rate (normalized current).

A.3 RK4 Discretization for the 1RC States

We discretize (11)–(12) with a fourth-order Runge–Kutta method. Let

$$x_k = \begin{bmatrix} v_{RC,k} \\ SOC_k \end{bmatrix}, \qquad f(x, I) = \begin{bmatrix} -\frac{1}{R_1 C_1} v_{RC} + \frac{1}{C_1} I \\ -\frac{I}{Q_{\text{nom}}} \end{bmatrix}.$$

For sampling period Δt,

$$k_1 = f(x_k, I_k), \tag{19}$$
$$k_2 = f\big(x_k + \tfrac{\Delta t}{2} k_1, I_{k+1/2}\big), \tag{20}$$
$$k_3 = f\big(x_k + \tfrac{\Delta t}{2} k_2, I_{k+1/2}\big), \tag{21}$$
$$k_4 = f(x_k + \Delta t\, k_3, I_{k+1}), \tag{22}$$
$$x_{k+1} = x_k + \frac{\Delta t}{6}\big(k_1 + 2k_2 + 2k_3 + k_4\big), \tag{23}$$

where $I_{k+1/2} = (I_k + I_{k+1})/2$.

A.4 Residual, Jacobian, and Gauss–Newton / LM Update

At each sample k, define the voltage residual

$$r_k(\theta) = V_{\text{model},k}(\theta) - V_{\text{meas},k}, \tag{24}$$

where θ collects the parameters of the multiplicative model (13) (e.g., $R_{0,\text{ref}}, E_a, \beta_1, \beta_2, \gamma_1, \kappa_1, \kappa_2$).

The scalar objective is

$$J(\theta) = \frac{1}{2} \sum_{k=0}^{N-1} r_k(\theta)^2. \tag{25}$$

Because R_0 enters (10) only algebraically (and R_1, C_1 are fixed), the Jacobian entries reduce to

$$\frac{\partial r_k}{\partial \theta_p} = -I_k \frac{\partial R_0}{\partial \theta_p}, \tag{26}$$

with R_0 given by (13). Differentiating (13) yields, for example:

$$\frac{\partial R_0}{\partial R_{0,\text{ref}}} = F_T F_{SOC} F_{SOH} F_C, \tag{27}$$
$$\frac{\partial R_0}{\partial E_a} = R_{0,\text{ref}}\, F_T F_{SOC} F_{SOH} F_C\, \frac{1}{R_g} \left(\frac{1}{T} - \frac{1}{T_{\text{ref}}} \right), \tag{28}$$
$$\frac{\partial R_0}{\partial \beta_1} = R_{0,\text{ref}}\, F_T F_{SOH} F_C\, (1 - SOC)^2, \tag{29}$$
$$\frac{\partial R_0}{\partial \beta_2} = R_{0,\text{ref}}\, F_T F_{SOH} F_C\, SOC^2, \tag{30}$$
$$\frac{\partial R_0}{\partial \gamma_1} = R_{0,\text{ref}}\, F_T F_{SOC} F_C\, (1 - SOH), \tag{31}$$
$$\frac{\partial R_0}{\partial \kappa_1} = R_{0,\text{ref}}\, F_T F_{SOC} F_{SOH}\, |C_r|^{\kappa_2}, \tag{32}$$
$$\frac{\partial R_0}{\partial \kappa_2} = R_{0,\text{ref}}\, F_T F_{SOC} F_{SOH}\, \kappa_1 |C_r|^{\kappa_2} \ln |C_r|. \tag{33}$$

(In practice, $\ln|C_r|$ is set to 0 when $|C_r|$ is below a small threshold.)

Stacking all samples yields a Jacobian $J \in \mathbb{R}^{N\times m}$ with rows (26). A Gauss–Newton step solves

$$(J^\top J)\,\Delta\theta = -J^\top r, \tag{34}$$

while Levenberg–Marquardt (LM) adds a damping term:

$$(J^\top J + \lambda I)\,\Delta\theta = -J^\top r. \tag{35}$$

In the special case where only a single scalar parameter (e.g., an effective $R_{0,\mathrm{ref}}$) is updated, (35) reduces to

$$\Delta R_0 = -\frac{\sum_k I_k r_k}{\sum_k I_k^2 + \lambda}. \tag{36}$$

The updated parameter is then

$$R_{0,\mathrm{ref,new}} = R_{0,\mathrm{ref}} + \Delta R_0. \tag{37}$$

A.5 Relation to the Proposed Neural ODE DCIR Framework

This 1RC baseline is useful to:

- quantify how much of the DCIR behavior can be captured by a single-pole ECM with hand-crafted $R_0(T, SOC, SOH, C_r)$,
- show that multi-time-constant diffusion and strongly transient regimes require a 2RC backbone and a residual model,
- demonstrate that, even with sophisticated parameterization and LM optimization, 1RC remains structurally incapable of reproducing two-slope relaxation and window-independent DCIR.

In contrast, the main body of this paper formulates DCIR estimation as a Neural-ODE problem with:

- a 2RC ECM backbone,
- temperature-aware neural parameter heads,
- a small residual network that learns only unmodeled dynamics,
- end-to-end training through a differentiable RK4 integrator.

The 1RC LM-based estimator should therefore be interpreted as a *classical reference*, not as a competing modern solution.