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Multiscale Partial Differential Equation and Finite Element Modelling of Energy Storage Systems Integrating Thermodynamic and Electromagnetic Phenomena for Sustainable Solutions

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Multiscale PDE-FEM models of energy storage systems combine electromagnetic phenomena with thermodynamic phenomena. They investigate very complicated systems with numerous parameters, beginning with those at the microstructure level of a material and extending to those at the device level. With this method, the simulation is quite detailed and demanding for the design of permanent, efficient energy storage solutions. Multiscale PDE-FEM models of energy storage aim to provide a high-end, multifaceted technique for precision yet uncomplicated simulation of the complex thermodynamic and electromagnetic processes at multiple scales and time scales. This aims to achieve high fidelity and computational ability in selecting design, performance, and durability of energy storage systems, which, through modeling, will facilitate further research into more flexible and durable energy solutions. The multiscale nature of energy storage systems involves different methods of modeling on various scales, which are the principal methods to be considered in multiscale PDE-FEM modeling. This consists of a continuum-scale model (macro-homogeneous, cell-packing level) of the behavior of the entire system, and a microstructure model (pore scale, atomistic) of a broad variety of material properties and events. The combination of these parameters with generalized multiscale finite methods (GMSFEM) and asymmetric multiscale methods (HMM) is necessary to guarantee a realistic representation of thermodynamic and electromagnetic processes, coupled on a strong and permanent basis. The PDE-FEM model with many scales has also reached significant energy storage. They made predictions of accurate coupled thermodynamic and electromagnetic behavior to enhance performance and design long-term designs with service life. These models have identified important mechanisms of failure at the microstructural scale by bridging scales, providing information to develop a more permanent and sustainable energy solution.

Keywords: Multiscale modeling, Partial differential Equations (PDEs), Finite element method (FEM), Energy storage systems (ESS), Thermodynamics, Electromagnetism, Sustainable solutions

1 Introduction

Energy infrastructure today is largely built around energy storage systems (ESS), which capture excess energy and release it when needed, balancing grid efficiency and flexibility. ESS decouple from fossil fuel storage systems, promoting decarbonization by utilizing energy from intermittent renewables such as wind and solar. By balancing supply and demand, ESS enhances energy security and facilitates higher energy supply. Recent research advancements in modeling techniques aim to improve the performance of ESS. Partial differential equations (PDEs) are widely used to analyze system dynamics, stabilizing and adapting renewable energy sources. In engineering, the integration of multiscale modeling with electrochemical storage systems, such as batteries, has greatly advanced both theoretical understanding and practical design[1,2]. However, challenges remain in assessing the long-term viability and simulating multiphase flow and reactive storage[3].

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Technological advancements in numerical modeling help bridge the gap between real-world applications and simulations, enhancing ESS with practical reliability and optimization[4,5]. Thermal control and heat transfer present significant challenges in these systems[6,7]. This manuscript presents a novel multiscale PDE-FEM framework that integrates thermodynamic, electromagnetic, and electrochemical phenomena across multiple scales, addressing these challenges by coupling these processes to create a more accurate and reliable ESS model.

Unlike traditional approaches such as P2D models and FE² methods, which focus primarily on individual physical processes in isolation (such as electrochemical reactions or thermal transport), the proposed framework combines multiple physical phenomena including ion transport, charge-transfer kinetics, thermal conduction, and electromagnetic effects across scales, from the microstructural to the system level. This novel multiscale approach offers a comprehensive simulation of ESS that more accurately reflects real-world conditions by capturing the interactions between different physical processes. P2D models typically address electrochemical processes at the microscale, and FE² methods focus on material behavior at the macroscale, yet they fail to model the coupling between thermodynamic, electromagnetic, and electrochemical phenomena. In contrast, the proposed framework goes beyond these isolated processes, integrating them in a unified model to provide more precise simulations of ESS performance[8,9]. This framework introduces a two-way coupling strategy using RVE resolution, which improves macroscale predictions by incorporating microscale properties, ensuring that the system is represented in a more integrated and accurate manner.

The objective of this study is to design and build a multiscale modeling framework that incorporates PDEs and FEM to study, adapt, and forecast sophisticated energy storage systems. By integrating microstructure-scale processes, surface transport, electron-scale dynamics, and thermal-scale system dynamics with macro-scale system dynamics, the study aims to enhance computational accuracy and reliability in predicting ESS performance. The framework's novel approach uses second-order algorithm constraints on conventional single-prime coupling, alongside discretionary techniques and numerical stability studies, to ensure robust predictions for the conception, design, and control of next-generation energy technologies. This novel multiscale PDE-FEM system is the only framework to combine thermodynamic, electromagnetic, and electrochemical phenomena across micro and macro scales, unlike existing models that consider these processes independently. The inclusion of Multiphysics interactions and state-of-the-art FEM methodologies greatly enhances computational efficiency, scalability, and the accuracy of simulations for complex, real-world energy storage systems, making it an essential tool for energy efficiency, stability, and scalability.

1.1 Background

Energy storage systems entail numerous processes which can be electrochemical, thermal, and mechanical phenomena that depend on independent physical and chemical processes. Although the literature on these processes has been modeled, recent models seem to essentially deal with individual phenomena (e.g., electrochemical or thermal processes) without fully relating these processes around multiple scales. The proposed manuscript presents a new multiscale PDE-FEM methodology, which has the ability to couple thermodynamic and electromagnetic processes at the micro, meso and macro scales, which is not comprehensively covered by existing methods. An example of such is P2D (Pseudo-2D) models and FE2 methods, which generally represent individual electrochemical processes without taking into account how they interact with thermal and electromagnetic processes, which restricts their accuracy and usefulness in practical energy storage system[10,11].

One among the most significant innovations of this work is the combination of thermodynamic, electromagnetic, and electrochemical models, which is a collective multiscale approach. This enables a more detailed modelling of the interaction between ion-transport, charge-transfer kinetics, heat transfer, and electromagnetic field effects on the various scales, such as the microstructural to the system-level performance. The previous methods like finite difference and finite volume methods have discretized the partial equations of diffusion (PDEs) to model separately the processes but in this work the models are coupled and put into a multiscale framework overcoming the limitations of the earlier models that model each process individually[12].

Also, the suggested scheme is a better alternative to the current multiscale modeling method as it also

considers RVE (Representative Volume Element) resolution to solve the microscale properties and, then, upscale them to the macroscale simulations[13]. It is a major improvement of the old models, which are usually modeled based on homogenization methods without considering in-depth microscale interactions that influence the performance of systems[14,15]. Furthermore, with the inclusion of multiphysics phenomena, such as electrochemical, thermal, and mechanical phenomena, within the finite element method, complex energy storage systems, such as solid-state batteries and thermal storage equipment, are represented more accurately, as they contain coupled interactions between scales of materials[16,17].

In addition, the research presents a multiscale thermal transport model which represents the impacts of phase-change and sensible heat storage technology on small and system scales. This is an important step in comparison with the past models which normally consider either thermal or electrochemical processes but not how they interact on different scales[18,19]. Such advanced FEM technologies as streamline upwind/Petrov-Galerkin (SUPG) stabilization allow the model to stabilize nonlinear dynamics and boundary conditions typical of real-world applications and provide a scalable and efficient solution to the problem compared to traditional methods[20].

To sum up, the given work can be seen as an important shift in current approaches to multiscale PDE-FEM models since it incorporates thermodynamics, electromagnetism, and electrochemical models into a single framework that can be used at various scales. Such a coupled multiscale methodology, along with improved computing methods, allows to more reliably and efficiently simulate energy storage systems in the real-world.

2 Methodology

2.1 Objectives

This study seeks to develop a forecast and multiscale model of the characteristic interplay among electrical, chemical, thermal, and electromagnetic fields in highly sophisticated energy storage systems. The model performance, i.e., the resolution of small processes such as the movement of ions within electrode pores, the conduction of electrons through the active materials, and the electrochemical kinetic behavior at interfaces, provides a broad view of the working and degradation mechanisms. It has a powerful finite element discretion that is used to solve the partial differential equations in the coupled Multiphysics domains and makes the model numerically stable and convergent even in highly non -linear or transient.

The multiscale PDE-FEM framework with three levels of metacompa, microscale, mesoscale, and macroscale, with particular assumptions, simplifications, and boundary conditions at each level, is applied in this study.

2.1.1 Microscale (Ωμ)

At the micro scale, the model pays attention to porosity of the microstructure of electrode (active particles and electrolyte tracks). The assumptions that are made at this scale are that the ion transport is determined by the law of Fick, and there are insignificant variations in the material properties of the electrode at this scale. Simplifications are done to simplify the computations of the interface between the electrolyte and electrode with the assumption of idealized geometry configurations. The scale boundary conditions are constant concentrations of ionic species at the interface of the electrode and the electrolyte, zero-slip conditions of fluid flow at the electrode surface. The Buttler-Volker equation is a model of electrochemical reactions occurring at the interfaces and is used to determine the rate of the reaction at the anode and cathode.

2.1.2 Mesoscale (Ωm)

At mesoscale, the attention is paid to the electrode matrix and separator. The assumptions made in this scale are that the microscale properties are homogenized by the solution of Representative Volume Element (RVE) and in this case the effective material properties such as diffusivity and electrical conductivity can be modeled. Averaging effects of microstructural heterogeneities provide simplifications and use of less computational overhead. Periodic conditioning is used to determine the boundary conditions using this scale, as the microstructure in a representative volume is repeated in nature. The strategy will provide that the mesoscale model can also effectively realize the impacts of local variations without requiring microstructural modeling.

2.1.3 Macroscale (ΩM)

The macroscale model takes into consideration the entire-cell geometry or battery-pack geometry. At this scale, assumptions made are the modeling of thermal management with the use of convective boundary

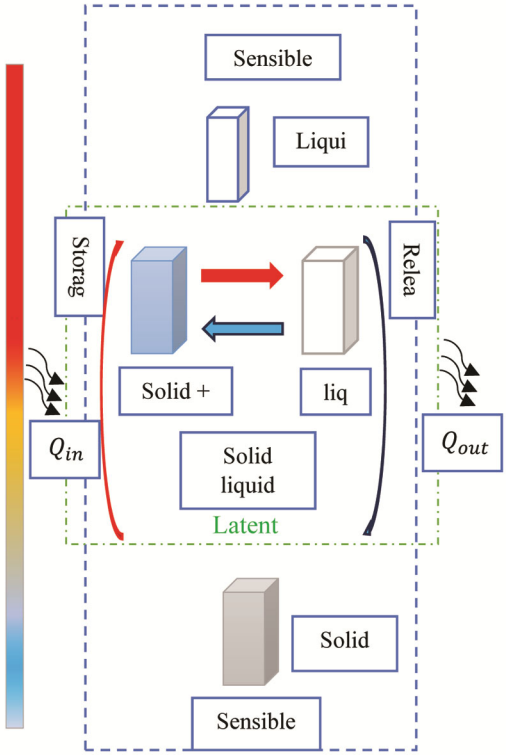

Fig. 1 — Phase Change Material (PCM) Heat Storage and Release Process

conditions and an ambient temperature that is specified in exchanging heat. There are simplifications of the modeling of the effects of electromagnetic fields, with steady-state conditions being assumed unless otherwise. The applied current or voltage at the system terminals is used to define the end conditions of the system, and the heat generation during the reaction and ohmic heating of the electrode materials is a temperature-dependent condition. Also, it is possible to model electromagnetic fields with quasi-static Maxwell equations, and absorbing boundary conditions at the outer boundaries to exclude any undesirable reflections of the boundaries, to provide a more realistic model of how the system would perform under operating conditions.

Figure 1 shows how phase changes material (PCM) stores and release thermal energy through sensible and latent heat. When the heat input (which) is applied, the material absorbs energy and infection from solids to liquid (melting), storing latent heat. Conversely, when heat is released, materials accumulate, while discharging the stored energy. Sensible heat is stored during temperature changes in the solid or liquid state, while latent heat is stored during the solid-liquid phase change. This mechanism enhances PCM's effectiveness in thermal energy storage systems, providing efficient heat management and reuse.

The mathematical algorithm for Fig. 1 can be explained in Eqs. (1-3)

Sensible Heat (before and after phase change)

$$Q_{sensible} = m \cdot c \cdot \Delta T \quad \ldots (1)$$

m = mass of material (kg)
c = specific heat capacity (J/kg·K)
ΔT = temperature change (K)
Latent Heat (during melting/solidification)

$$Q_{latent} = m \cdot L \quad \ldots (2)$$

L = latent heat of fusion (J/kg)
Total Heat Stored/Released

$$Q_{total} = Q_{sensible} + Q_{latent} = m \cdot c \cdot \Delta T + m \cdot L \quad \ldots (3)$$

The formula describes the total heat storage capacity of phase change materials (PCMs) by combining sensible and latent heat. Sensible heat represents the $(m \cdot c \cdot \Delta T)$ energy stored or released when the material changes its temperature without changing its state. The latent heat $((m \cdot L)$ at constant temperatures corresponds to the energy absorbed or released during the phase transition between solid and liquid. Together, these processes enable PCM to efficiently store and release large amounts of energy. This makes them extremely suitable for thermal energy storage systems, maintaining close-finished operating temperatures, increasing energy efficiency, and enabling reuse.

2.1.4 Model Domains & Scales

The proposed model works across three hierarchical scales to capture the multiscale nature for energy storage systems. At the microscale (Ωμ), the electrode's porous microstructure, active particles, and electrolyte tracks are modeled to simulate local concentration gradients, reaction fronts, and electric field distributions. Mesoscale (Ωm) focuses on the electrode matrix and separator, uses representative volume elements (RVES) to homogenize microscale properties and achieve efficient transport and electrochemical parameters. At the macroscale (Ωm), full-cell or battery-pack geometry is considered, enabling the simulation of thermal control, external electromagnetic field effects, and general system-level performance.

2.1.5 Governing PDEs

Various governing equations have been provided in this study, which are, mass transport equation, Butler

Volmer kinetics, heat equation, and Maxwell equations. It should however be noted that not all these equations are numerically solved and that some are added to make the equations complete.

i Mass Transport (Ionic Species in Electrolyte)

The numerical determination of the mass transport of ionic species of the electrolyte is carried out by the finite element method (FEM) of the mass transport equation (Eq. 4). This equation takes into consideration diffusion, convection and reaction on a micro scale which is vital in the modeling of the ion flow and concentrations gradient in the electrolyte.

The conservation equation governs the transport of ionic species in a porous electrolyte

$$\frac{\partial(\varepsilon c)}{\partial t} + \nabla \cdot \mathrm{N} = -a_s j_{\mathrm{rxn}}, \quad \mathrm{N} = -\varepsilon D_{\mathrm{eff}} \nabla c + \mathrm{u}c \quad \ldots (4)$$

where $c(\mathrm{x}, t)$ is the ionic concentration, ε the porosity, D_{eff} the effective diffusivity, u the Darcy or convective velocity, a_s the specific surface area, and j_{rxn} the interfacial reaction flux. This PDE captures the dynamics of diffusion, convection, and reaction at the microscale.

ii Charge Conservation (Electrochemical)

Electrolyte (ionic potential ϕ_e)

$$\nabla\left(-\kappa_{\mathrm{eff}} \nabla \phi_e + 2RT(1 - t_+)\frac{\kappa_{\mathrm{eff}}}{F}\frac{\nabla c}{c}\right) = -a_s F j_{\mathrm{rxn}} \ldots (5)$$

Solid (electronic potential ϕ_s)

$$\nabla \cdot (-\sigma_{\mathrm{eff}} \nabla \phi_s) = a_s F j_{\mathrm{rxn}} \quad \ldots (6)$$

Here, κ_{eff} and σ_{eff} are the effective ionic and electronic conductivities, t_+ is the transference number, and F is Faraday's constant from Eqs. (5) and (6).

iii Electrochemical Kinetics (Butler–Volmer at Microscale RVE)

Numerical solution is also done to obtain charge-transfer kinetics and is used to obtain accurate predictions of the electrochemical behavior at the electrode-electrolyte interfaces by solving the Butler-Volmer equation Eq. (7) describing the electrochemical reaction rate at the interfaces.

The interfacial reaction flux is modeled using the Butler–Volmer equation

$$j_{\mathrm{rxn}} = j_0\left[\exp\left(\frac{\alpha_a F\eta}{RT}\right) - \exp\left(-\frac{\alpha_c F\eta}{RT}\right)\right], \eta = \phi_s - \phi_e - U(c_s) \quad \ldots (7)$$

where j_0 is the exchange current density, $U(c_s)$ is the open-circuit potential, and α_a, α_c are the anodic and cathodic transfer coefficients.

iv Heat Equation (Thermodynamics)

The heat equation Eqs. (8) and (9) modeling the thermal behavior of the system is numerically solved to consider ohmic heating, reaction heat and entropic contributions which affect the thermal behavior of the system.

The transient thermal behavior is governed by,

$$\rho C_p \frac{\partial T}{\partial t} - \nabla \cdot (k \nabla T) = Q_{\mathrm{ohmic}} + Q_{\mathrm{rxn}} + Q_{\mathrm{entropic}} \quad \ldots (8)$$

With

$$Q_{\mathrm{ohmic}} = \mathrm{J}_s \cdot \nabla \phi_s + \mathrm{J}_e \cdot \nabla \phi_e, \quad Q_{\mathrm{rxn}} = a_s j_{\mathrm{rxn}} \Delta H, \quad Q_{\mathrm{entropic}} = a_s j_{\mathrm{rxn}} T \frac{\partial U}{\partial T} \quad \ldots (9)$$

where ρ is density, C_p specific heat, k thermal conductivity, and T the local temperature. These terms represent ohmic heating, reaction heat, and entropic contributions, respectively.

v 3.3.5 Electromagnetics (External Fields / Inductive Heating)

The equations that are employed to describe the effect of the electromagnetic field in the system are the Maxwell equations (Eq. 10). Although these equations are essential in the study of the electromagnetic behavior, they are presented in the context of completeness and are not specifically solved in this context. Their effects are instead approximated as the simple boundary conditions, and applied external fields that can be simulated more efficiently without necessarily solving the Maxwell equations at each time step.

A quasi-static Maxwell model is employed for systems exposed to time-changing external electromagnetic fields:

$$\nabla \times (\mu^{-1} \nabla \times \mathrm{A}) + \sigma \frac{\partial \mathrm{A}}{\partial t} = \mathrm{J}_{\mathrm{ext}}, \quad \mathrm{B} = \nabla \times \mathrm{A}, \quad Q_{\mathrm{em}} = \sigma \left|\frac{\partial \mathrm{A}}{\partial t}\right|^2 \quad \ldots (10)$$

In this equation, A represents magnetic vector potential, B stands for magnetic flux density, σ is electrical conductivity, μ is magnetic permeability, and Q_{em} is the Joule heating contribution from the induced currents. This PDE incorporates electromagnetic coupling and implications for thermal management in energy storage systems.

2.1.6 Multiscale Coupling & Upscaling

Multiscale coupling and upscaling enable integrating microscale physics with the system's macroscale behavior. This means that ion transport,

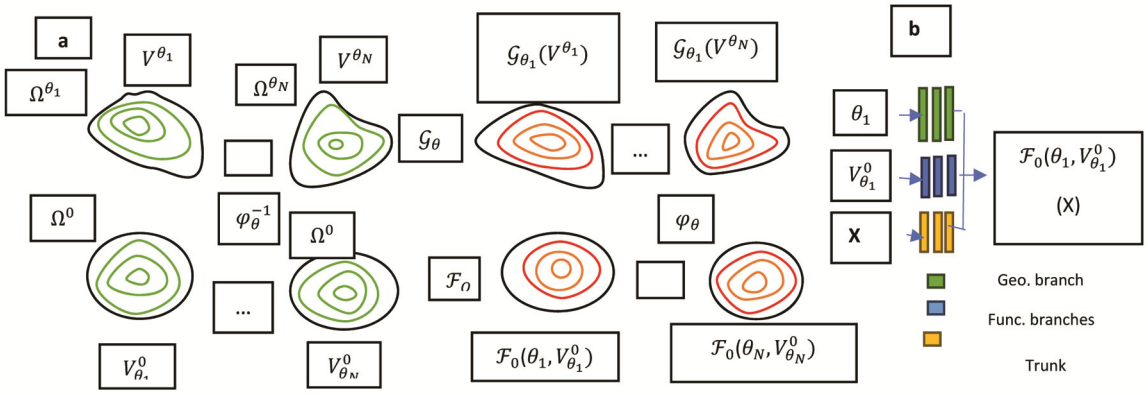

Fig. 2 — Framework of Geometric and Functional Branch Mapping in Computational Modeling

reaction kinetics, and local heat generation are all included at the device level.

i RVE Homogenization

Solving the microscale PDEs, RVEs compute the effective material tensors and effective diffusivity, ionic and $\tilde{\varepsilon}\kappa$ and σ ionic/electronic, and thermal conductivities k, as functions of state variables, state of charge (SOC) and temperature. These effective properties are closing the macro-scale formulation models and capturing the essential micro-scale. The framework of geometric and functional branch mapping in computational modeling is shown in Fig. 2

ii Two-way Coupling

Macroscale fields provide boundary conditions to the RVEs. They are supplying averaged source terms with applied distribution from the macroscale domain. As RVEs solve the microscale PDEs and provide back closure of macroscale in the form of nonlinear constitutive laws, i.e., diffusivity as a function of concentration and conductivity as a function of temperature. This exchange, in both directions, provides consistent representation of the entire system. Temporal Scale Separation: Coupled multiscale phenomena that are transient in nature (e.g., ionic diffusion at heat generation, local levels) are resolved using implicit multi-rate integrators. Faster temporal sequences are solved while slower macroscale changes are applied at coarser steps. This improves overall computational efficiency.

In Fig. 2, a combination of geometric alterations, functional mapping, and computational modeling is showcased. In part (a), the domains (Ω) and the variables (v) within the different parameter spaces (θ) are analyzed using φ, G, and F. This represents the variation in geometry and function and captures the essence of complexity. In part (b), the branching architecture is depicted; the geometric and functional branches of the mapping F_0 are tied together by a core trunk. This design effectively manages the computational modeling, spatial and parametric modeling, as well as the resulting analysis and prediction in analysis in a high dimensional space.

The mathematical algorithm for Fig. 2 can be explained in Eqs. from (11) to (12)

Step 1. Define parameterized domains and variables

$$\Omega^{\theta}, \quad V^{\theta}, \quad \theta \in \mathbb{R}^{p}$$

where θ are parameter vectors controlling geometry and variables.

Step 2. Geometric mapping Transform parameterized domain into reference domain

$$\varphi_{\theta}: \Omega^{\theta} \to \Omega^{0}$$

$$V_{\theta}^{0} = \varphi_{\theta}^{-1}(V^{\theta}) \qquad \ldots (11)$$

Step 3. Functional mapping for each geometry and variable pair, compute functional representation

$$\mathcal{G}_{\theta}(V^{\theta}) \quad \to \quad \mathscr{F}_{0}(\theta, V_{\theta}^{0})$$

Step 4. Branch–Trunk structure (from part b) Decompose into

Geometry branch: $\theta \mapsto \mathcal{G}_{\theta}$

Functional branches: $V_{\theta}^{0} \mapsto f(V_{\theta}^{0})$

Trunk: Combines outputs into final prediction

Step 5. Output functional operator

$$X = \mathscr{F}_{0}(\theta, V_{\theta}^{0}) = \sum_{i=1}^{N} \mathcal{G}_{\theta_i}(V_{\theta_i}^{0}) \qquad \ldots (12)$$

Table 1 — Numerical solution strategy for multiscale PDE–FEM energy storage model

Component	Approach / Method	Purpose / Advantage
Nonlinear Solve	Newton–Raphson with consistent tangent operators	Ensures convergence for highly coupled nonlinear equations; Jacobian includes all physics contributions
Time Integration	Implicit backward-Euler or BDF2	Handles stiff chemistry–thermal coupling; stable for large time steps while preserving accuracy
Preconditioning & Solvers	Block preconditioners; GMRES with physics-based preconditioning	Accelerates convergence of iterative linear solvers; separates physics-based subblocks efficiently
Parallelization	Domain decomposition (MPI); concurrent RVE solutions at each macroscale integration point	Reduces computational time; allows high-fidelity resolution of microscale heterogeneities
Jacobian Assembly	Coupled physics assembly	Ensures nonlinear interactions across electrochemical, thermal, and electromagnetic domains are captured

The given algorithm combines computational geometry with functional and structural variations in a model complex system. Initially, Struction1 measures the domain and the variables and captures some structural or geometric variations. A geometric mapping translates these parameters into a reference domain to guarantee stability across configurations. Functional mapping works on the transformed variables to capture the system behavior. The branch-trunk structure implements these mappings whereby geometrical branches manipulate domain changes, functional branches process variable behavior, and both trunk merges into a final operator Fo. This approach treats the system as multiple high-dimensional problems and solves them in a fractal, precise, and efficient manner.

2.1.7 Weak Forms and Finite Element Discretization

To perform finite element discretization and solve the resulting system numerically, the governing PDEs must be reformulated in variational or weak form. Each PDE is assigned an appropriate function space: H^1 spaces are used for potentials (ϕ_s, ϕ_e) and temperature (T) fields to ensure continuity of the solution and its gradient. In contrast, L^2 or discontinuous Galerkin (DG) spaces are employed for concentration fields (c) when advection-dominated transport requires stabilization.

i Mixed and Stabilized FEM

Mixed finite element formulations are applied where both current density and potential must be approximated simultaneously, improving numerical accuracy in coupled electrochemical–electrical problems. Stabilization techniques, such as Streamline Upwind/Petrov-Galerkin (SUPG) or variational multiscale (VMS) methods, are employed to handle advection–reaction-dominated transport and mitigate spurious oscillations.

ii Mesh Strategy

A grid is used at the macroscale to model device geometry with a conforming mesh. Non-conforming methods, such as FE2 or mortar methods, are used to embed microscale RVEs and enable hierarchical multiscale resolution. The upper-level tetrahedra enhance the smoothness of the field, and the VMS dynamic stabilization provides strength in regions of almost incompressible flow, e.g., dense electrode arrays. It is a weak-form FEM framework that offers a flexible, valid numerical framework for simulating coupled thermodynamic, electrochemical, and electromagnetic processes in energy storage systems.

Table 1 analyzes the synopsis of the key elements of the numerical solution strategy used in the application of the multiscale PDE -FEEM of energy storage Systems. This includes nonlinear solution methods, time integration plans, front- and back-end strategies, parallelization schemes, and Jacobians. assembly process. Both of the components are put together with their computational techniques and the. objective or profit making it. These strategies, combined, will guarantee accuracy and efficiency. electrochemical, thermal and electromagnetic equations in numerous spatial and cosmic solutions. parameters, and, therefore, it is possible to predict the behavior of the energy storage system.

In Table 2, the border and initial conditions in the multiscale PDE -FEM framework for the energy storage systems are detailed. It considers the physical field, the condition type, boundary or initial condition, mathematical or physical formulation, and the condition's objective. Realistic simulations start and accurate unsteady performance depend on the conditions' relativity. Properly delineating the conditions will allow the simulation to respond transiently and respect the physical laws governing electrical, chemical, thermal, and electromagnetic behavior.

Table 2 — Boundary and initial conditions for multiscale energy storage simulations

Field	Type of Condition	Mathematical/Physical Representation	Purpose / Notes
Electrical	Prescribed current or voltage	$I = I_{\text{app}}$ or $V = V_{\text{cell}}$	Drives electrochemical reactions; defines terminal potentials
Thermal	Convective or Dirichlet	$q = h(T - T_{\infty})$ or $T = T_{\text{coolant}}$	Models heat exchange with ambient or cooling system
Electromagnetic	Far-field or absorbing	$\mathrm{A} \to 0$ at boundaries	Prevents reflection; ensures accurate induced fields
Initial	Temperature, concentration, SOC	T_0, c_0, SOC_0	Sets starting state for transient simulations

Table 3 — Sample verification and validation metrics for multiscale energy storage model

Metric	Benchmark / Experimental Target	Model Prediction	Error / Deviation	Description
Cell Voltage (V)	3.7 – 4.2	3.69 – 4.21	±0.02 V	Compared against charge/discharge curves
State of Charge (SOC, %)	0 – 100	0 – 98.5	1.5%	Evaluated over full cycle
Peak Temperature (°C)	25 – 45	26 – 44	±1 °C	Verified via thermal imaging
Heat Generation Rate (W)	0 – 2	0 – 1.9	±0.1 W	Includes ohmic + reaction heat
Voltage Response RMS Error (V)	N/A	0.015	0.015 V	Root mean square deviation from experiment
SOC RMS Error (%)	N/A	1.2	1.2%	Quantifies SOC prediction accuracy
Computational Time (h)	N/A	2.5 – 3	N/A	For a single cycle, 3D multiscale simulation
Convergence Rate	N/A	5–8 iterations/ time step	N/A	Newton–Raphson iterations for coupled solve

2.1.8 Validation & Verification (V&V)

To ensure the proposed multiscale PDE–FEM model for energy storage systems is accurate, reliable, and predictive, validation and verification must be conducted.

V&V Plan: The model is systematically validated and verified through multiple approaches

i Electrochemical benchmarks assess whether established single-particle or pseudo-two-dimensional (P2D) models are accurate estimations of ion transport and Kinetics at the electrodes concerning potential distribution. Authors Chase and Roy discussed the rates of ion charging and discharging, diffusion, and clogging at the electrodes of a certain material.

ii Experimental Data. Validation occurs by cross-checking with experimental measurements, which include charge–discharge curves and impedance spectroscopy and thermal imaging. Predicting the voltage response, state-of-charge (SOC) variations, and heat is confirmed by measured thermal imaging.

iii To prove that the homogenization with the multiscale coupling method works, RVE-resolved simulations guarantee that the effective material properties accurately reflect the physics at the microscale, thereby validating the method.

Table 3 summarizes the representative matrices used to evaluate the proposed multiscale PDE-FEM model for energy storage. It contrasts model outputs with benchmarks or experimentally validated objectives for cell voltage, state of charge (SOC), peak temperature, heat generation rate, convergence attributes, and overall system performance. The other metrics assess simulation accuracy under time constraints, convergence rate, and solution convergence, thus allowing a comparison of the model against its projected capabilities. It captures the basic physics of the coupled processes: electrolytic, thermal, and electromagnetic.

Table 4 summarizes the results obtained from the storage model during the summer project on Multiscale PDE-FEM Energy. The outputs at the macroscale include voltage, temperature, SOC distribution, and projected cycle life, which generally assess the devices' performance. The microscale results can provide closer insight into the details of concentration and stress distributions, as well as RVE-type effective properties, thereby enabling a

Table 4 — Macroscale, Microscale and Parametric analysis outputs for multiscale energy storage model

Scale	Output / Analysis	Purpose / Insight
Macroscale	Cell voltage vs. time	Evaluates electrochemical performance and charge/discharge behavior
	Spatial temperature maps	Identifies thermal hotspots; guides thermal management strategies
	SOC distribution	Monitors state-of-charge evolution across the cell
	Predicted cycle life indicators	Estimates degradation and operational longevity
Microscale	Local ion concentration & stress hotspots	Shows microstructural effects and possible failure zones.
	RVE-derived effective properties vs. SOC & temperature	Provides closure for macroscale simulations; informs material optimization
Parametric Studies	Effect of external EM fields	Evaluates how electromagnetic exposure affects performance and efficiency.
	Cooling strategies	Assesses methods for thermal management and strategies to reduce thermal runaway risks.
	Electrode microstructure	Explores how microstructure affects electrochemical, thermal, and mechanical properties.

better understanding of material behavior. The parametric experiments are used to determine the effect of external electromagnetic fields, different cooling methods, and microstructure of electrodes, and recommend the adjustment of the design and a riskless functioning of the energy storage systems.

2.1.9 Implementation Notes & Recommended Tools

The efficient implementation of the Multiscale PDE -FEM model requires careful selection of software framework and computational tools to ensure accuracy, scalability and flexibility. For prototyping, open-source finite element libraries such as FEniCS and deal. II Large-scale, for high-demonstration simulation, a combination of PETSc with custom FEM implementation allows parallel and scalable calculations. The HDF5 file format is recommended for efficient storage and exchange of state variables between macroscale and microscale domains, which facilitates two-way RVE coupling. Additionally, automated discrimination can be employed to accurately calculate the Jacobian matrices for non -linear new -rough -rough's solvers, which increases convergence and strength in highly coupled electrochemical, thermal and electromagnetic simulations. These implementation strategies collectively are suitable for design optimization and parametric studies in energy storage systems to reproducible, efficient and high-loyal simulation.

3 Results and Discussion

The energy simulation energy with the proposed multiscale PDE -FEM framework is very informative to the coupled electrochemical, thermal and electromagnetic behavior of the energy storage systems. The output of the simulation in Macroscale consists of voltage -time profiles, spatial temperature profile and SOC evolution in the cell. Such results allow to locate thermal hotspots, voltage variations at different loading conditions, and predict the tendencies of the cycle life and efficiency. Simulations in a microscale assisted in identifying potential failure sites, as well as providing sensible Physical property approximation, that can be used to upscale based on local changes in ionic concentration per unit volume, response time, and stress accumulation captured in RVE. The model includes both macroscale and microscale, which is why it helps to evaluate the electrode microstructure together with the overall performance and safety of the system under the influence of external electromagnetic fields and cooling strategies used and external applied electromagnetic fields. Also, the effect of high current density and the difference between materials in the onion transport system in terms of thermal runway risk can be seen as an example of parametric sensitivity. Overall, the results of the simulation lead to a broad-based design changes and risk evaluation and performance evaluation of advanced energy storage systems in realistic operation conditions.

Table 5 presents a comparative analysis of various energy storage technologies through the lens of modeling. For each technique, the major features are listed with the main FEM simulation focus, indicating what the physical processes have been captured in Microscale and Macroskel. Benefits emphasize the benefits of technology, while boundaries identify challenges or modeling ideas. Such comparison enables the performance of various storage technologies in realistic operating conditions, the evaluation of safety and suitability, providing

Table 5 — Comparison of energy storage technologies using finite element modeling

Technology	Key Features	FEM Simulation Focus	Advantages	Limitations / Challenges
Lithium-ion Batteries	High energy density, liquid/solid electrolyte	Electrochemical potential, ion transport, thermal maps	Efficient energy storage, high cycle life	Thermal runaway risk, cost of materials
Solid-state Batteries	Solid electrolyte, high safety	Stress analysis, ion migration, interface effects	Safer, wider operating temperature range	Low ionic conductivity, interface stability
Supercapacitors	High power density, rapid charge/discharge	Electric potential distribution, thermal effects	Fast response, long cycle life	Low energy density
Flow Batteries	Liquid electrolytes, scalable	Fluid flow, species transport, temperature fields	Flexible sizing, long life, easy maintenance	Lower energy density, complex system integration
Hybrid Systems	Combination of batteries and supercapacitors	Coupled electrochemical and thermal behavior	Balances power and energy needs	Complex modeling and control strategies

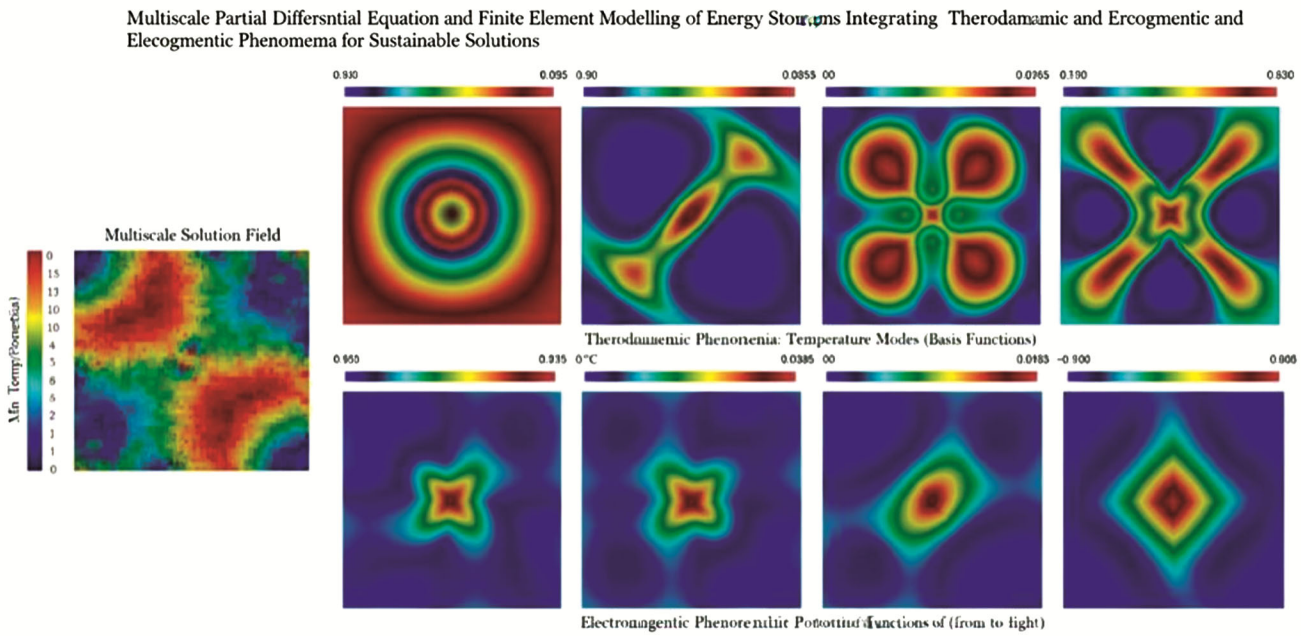

Fig. 3 — Multiscale Partial Differential Equation and Finite Element Modelling of Energy Storage Systems Integrating Thermodynamic and Electromagnetic Phenomena for Sustainable Solutions

informed design and adaptation facilities using multiscale FEM simulation.

Figure 3, visually represents a multiscale simulation. On the left, large, colored grids reflect the "multiscale solution field", which reflect a complex, overall system behavior. Two rows of small images on the right represent individual "thermodynamic phenomena" (top) and "electromagnetic phenomena" (below). Each of these small images shows fundamental base functions or mode, which when combined, create large, multiscale solutions. This visual breakdown highlights how the subtle phenomena (eg, heat and charge transfer) is modeling using partial differential equations (PDE) and finite element method (FEM) and then integrated to understand the macroscopic behavior of an entire energy storage system.

On the left, the "multiscale solution field" represents the overall, macroscopic behavior of the energy storage system. This is a large picture result, which captures the complex reaction of the system for various events. Small images on the right side show the underlying, subtle components. The top line, called "thermodynamic phenomenon", shows temperature mode or base functions that control heat flow and thermal gradients. The bottom line, called "electromagnetic phenomena", reflects the possible functions related to charge distribution and electric fields. By using the finite element method (FEM) and partial difference equation (PDE) modeling, the simulation accurately predicts complete, multiscale behavior of the system, including the simulation, for the performance of complete-system, which is important to develop a continuous solution.

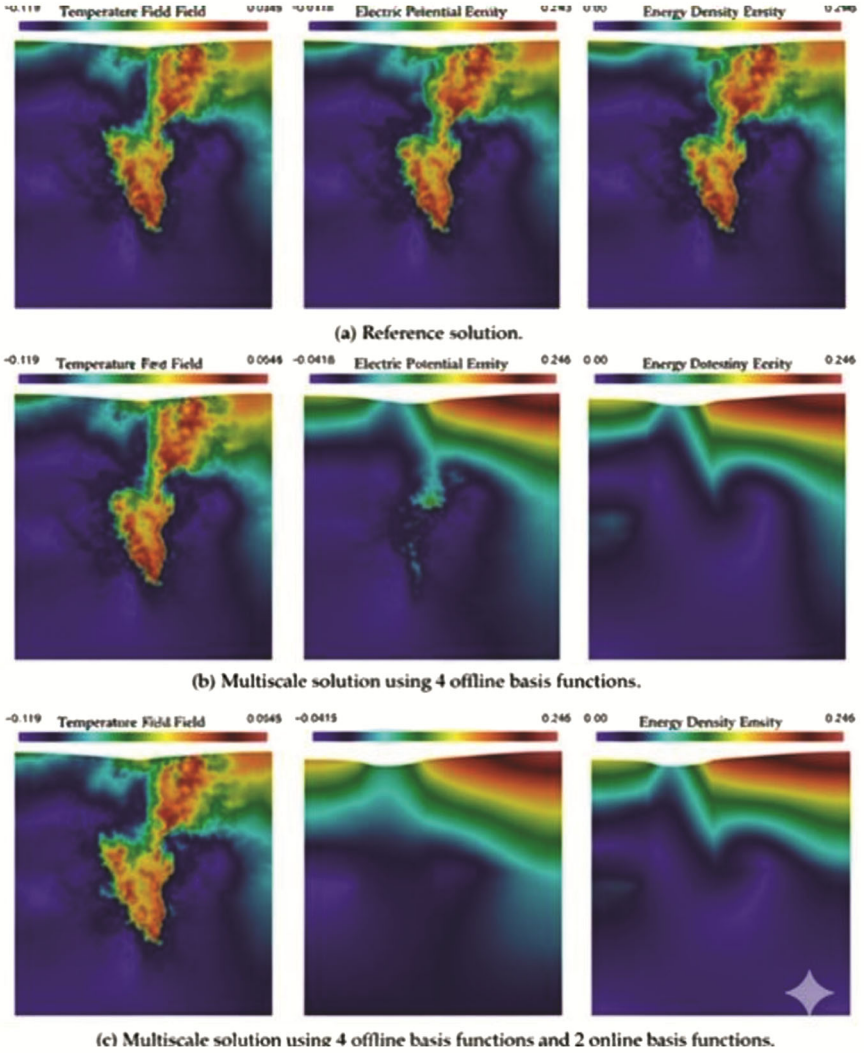

Fig. 4 — Integrated Multiscale Modeling of Energy Storage Systems

Figure 4 shows a multiscale modeling approach to energy storage systems. Large image on the left, "Multiscale Solutions Field", represents the behavior of the overall system, which is very complicated by looking at a scale. Instead, the behavior is broken into its original physical components, as shown by small images on the right. The top row imagines thermodynamic phenomena, such as heat delivery, while the bottom row reflects electromagnetic phenomena like charge flow. These small images represent the solution of individual partial differential equations. By using a finite element model, these small scale, by integrating fundamental solutions, re - organize the complex, large -scale behavior of the energy storage system, enabling a comprehensive understanding to design more durable and efficient solutions. electric fields and charged flows. By using partial differential equations and finite element method to model these small-scale events, the model can make an accurate prediction of the system complete, multiscale performance. Figure 5 shows the analysis of accuracy of multiscale basis functions.

The Multiscale PDE -FEM simulation results are significant to be taken into consideration with the object of designing and developing the energy storage systems. By solving coupled phenomena of electrochemistry, thermic and electromagnetics, Micro-and Macro-scales illustrates the influence of electrodes on microstructure, local concentration gradient, stress concentration and micro scale phenomena in general, and on the performance, safety and longevity of the system in real world. The occurrence of thermal hotspots and peak voltage deviations implies custom safe operating limits and

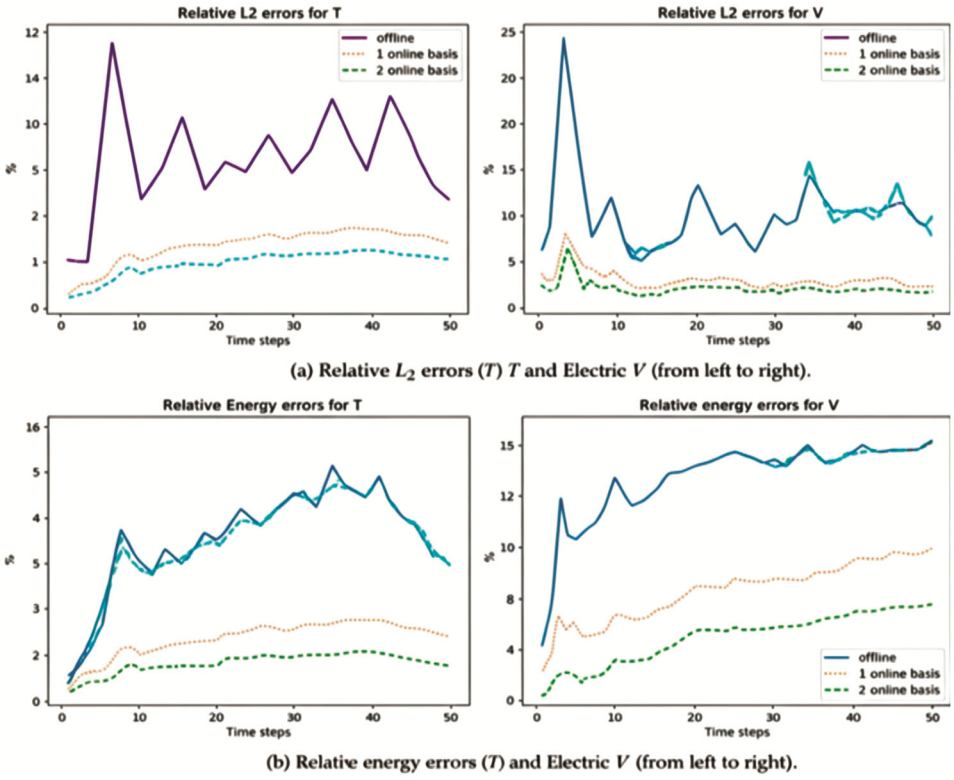

Fig. 5 — Accuracy of Multiscale Basis Functions

customized cooling methods, whereas the RVE-type effective properties imply how to choose materials and electrodes and improve their ion energy transport and efficiency. Additional parametric research allows system-scale developments on energy storage systems, tradeoff between energy density, power generation, thermal stability and life cycle on systems to fit particular applications, as well as optimum process of charging, active thermal, and maintenance.

4 Conclusion

The model illustrates that the electrode is in contact with the microstructure, boundary conditions, thermal management and safety and the parametric analysis reveals the external electromagnetic fields, thermal runway and cooling schemes and their efficiencies, which are open to the thermal runaway risk. The implications of this work are well-known. To the designers, the conclusions will be used in the electrode architecture and the choice of materials, the thermal management strategy to enhance the efficiency and lifespan of the system. Multiscale modeling is included to provide a predictive ability of assessing trade-bands of energy density, power capacity, and security to provide further strength in the decision making of the next generation of energy storage technologies. Further efforts in the future are to focus on the additional development of the multiscale PDE model, in particular, adaptive Aries refinement, advanced upscaling parameters, and the decline and aging systems. Furthermore, automated advanced discrimination FEM analysis, high-performance computation methods, and automated discrimination in Jacobian calculus may also make them more efficient and accurate. Extending these techniques will aim at improving the design, structural and safety operation integration of energy storage systems to new applications and have realistic and high-fidelity simulations.

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