International Research Training Group IRTG 2657
Computational Mechanics Techniques in High Dimensions

A Numerical Investigation of Granular Structure Influences on Battery Performance

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Project Overview

Modern lithium-ion battery cathodes are **granular composite materials**. Micro-structural features such as **porosity, tortuosity, and particle arrangement** critically affect electro-chemo-mechanical performance. Understanding their evolution during manufacturing is key to improved design and robust simulation pipelines.

Application Context: calendaring / compaction of cathode layers; link to multi-physics performance metrics in operation.

Methodology

Hybrid Continuum–Discrete Simulation

MPM–DEM hybrid

- A hybrid material point-discrete element method (MP-DEM) is used to simulate particle-scale interactions during the calendaring process of battery cathodes.

High-Fidelity Mesh Generation

PFEM-inspired technique

- The resulting granular assemblies are converted into 3D finite element meshes using a PFEM (Particle Finite Element) - inspired technique.

Multiphysics Finite Element Simulation

- Electrochemical response under charge/discharge cycles.
- Coupled electro-chemo-mechanical behavior.
- Stress distribution and deformation in the electrode.

Reduced Order Modeling (ROM)

Parametric Proper Orthogonal Decomposition (PPOD)

- Preserve key physical behaviors (electrochemistry, mechanics) across micro-structures.
- Enable rapid evaluation of performance metrics (capacity fade proxies, stress hot-spots).
- Compare ROM vs. FOM accuracy and speed; define validation benchmarks.

Mathematics of Model Generation

Carbon-Binder Domain (CBD) shell thickness

$$m = \sqrt[3]{r^3 + \frac{3\left(\frac{4}{3}\pi r^3\right)\left(\phi_{\mathrm{CBD}}/\phi_{\mathrm{AM}}\right)}{\Omega}} - r, \qquad \Omega = 2\pi\left(1 - \cos\theta\right)$$

m = CBD shell thickness, $\phi_{\mathrm{CBD}}/\phi_{\mathrm{AM}}$ = target volume ratio, Ω = cone solid angle, θ = cone half-angle.

MPM particle spacing and total number

$$d = \sqrt[3]{\frac{dx^3}{n_{\mathrm{mp}}}}, \qquad N_{\mathrm{MP,cone}} = \frac{\Omega}{3} \cdot \frac{(r+g+m)^3 - (r+g)^3}{d^3}$$

d = material point spacing, dx = base grid size, n_{mp} = MPs per cell, $N_{\mathrm{MP,cone}}$ = MPs per cone in the offset shell $[r+g,\ r+g+m]$.

Volume fractions in the simulation box

$$\phi_{\mathrm{AM}} = \frac{N_{\mathrm{core}} V_{\mathrm{AM}}}{V_{\mathrm{box}}}, \quad \phi_{\mathrm{CBD}} = \frac{N_{\mathrm{MP}} v_{\mathrm{MP}}}{V_{\mathrm{box}}}, \quad \phi_{\mathrm{pore}} = 1 - \phi_{\mathrm{AM}} - \phi_{\mathrm{CBD}}$$

ϕ_{AM} = AM volume fraction, ϕ_{CBD} = CBD volume fraction, ϕ_{pore} = remaining void space; V_{AM} = core volume, V_{box} = total domain volume, v_{MP} = volume per MP.

Model Generation

MPM–DEM Model and Experimental SEM Image:

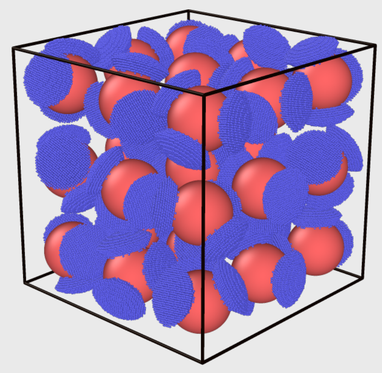

Figure 1: Computational modelling of electrode.

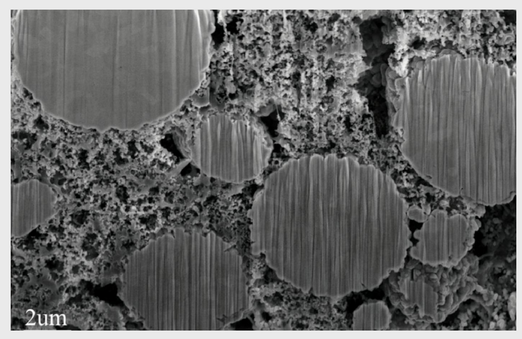

Figure 2: Cross sectional image of electrode [a].

Preliminary Results

MPM–DEM Model Load-Displacement Analysis:

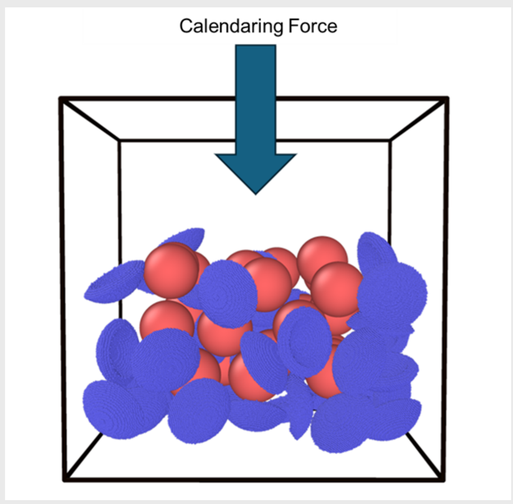

Figure 3: Computational model compaction.

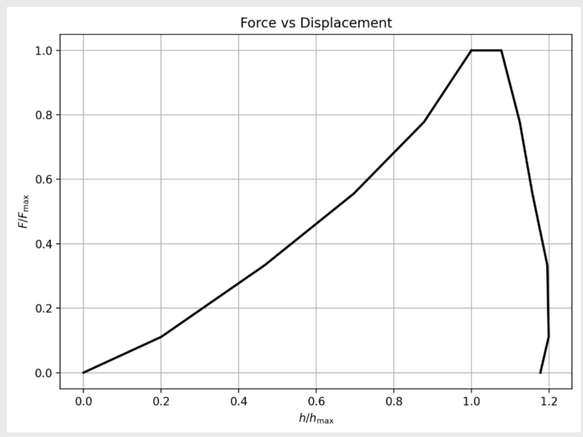

Figure 4: Force-displacement curve.

Publications and References

[1] Y. Jiang and A. **A. Tabak Cevit**, *Hybrid continuum–discrete simulation of granular structure evolution in battery electrodes during calendaring*, in preparation, 2025.

[2] **A. Tabak Cevit** and Y. Jiang, *Numerical investigation of the influences of constitutive models for the binder using continuum–discrete solver*, in preparation, 2025.

[3] **A. Tabak Cevit** and Y. Jiang, *Hybrid MPM–DEM framework for constructing computable mesh models of battery granular structure*, in preparation, 2025.

[a] R. Xu et al., *Heterogeneous damage in Li-ion batteries: Experimental analysis and theoretical modeling*, J. Mech. Phys. Solids, 129:160–183, 2019. doi:10.1016/j.jmps.2019.05.003.

IRTG Environment and Activities

- **Particles 2025:** (Barcelona, Oct 2025).
- **WCCM & ECCOMAS:** (Munich, Jul 2026).
- **Planned stay ENS Paris – Saclay:** January – June 2026.
- **Particles 2027:** (2027).

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