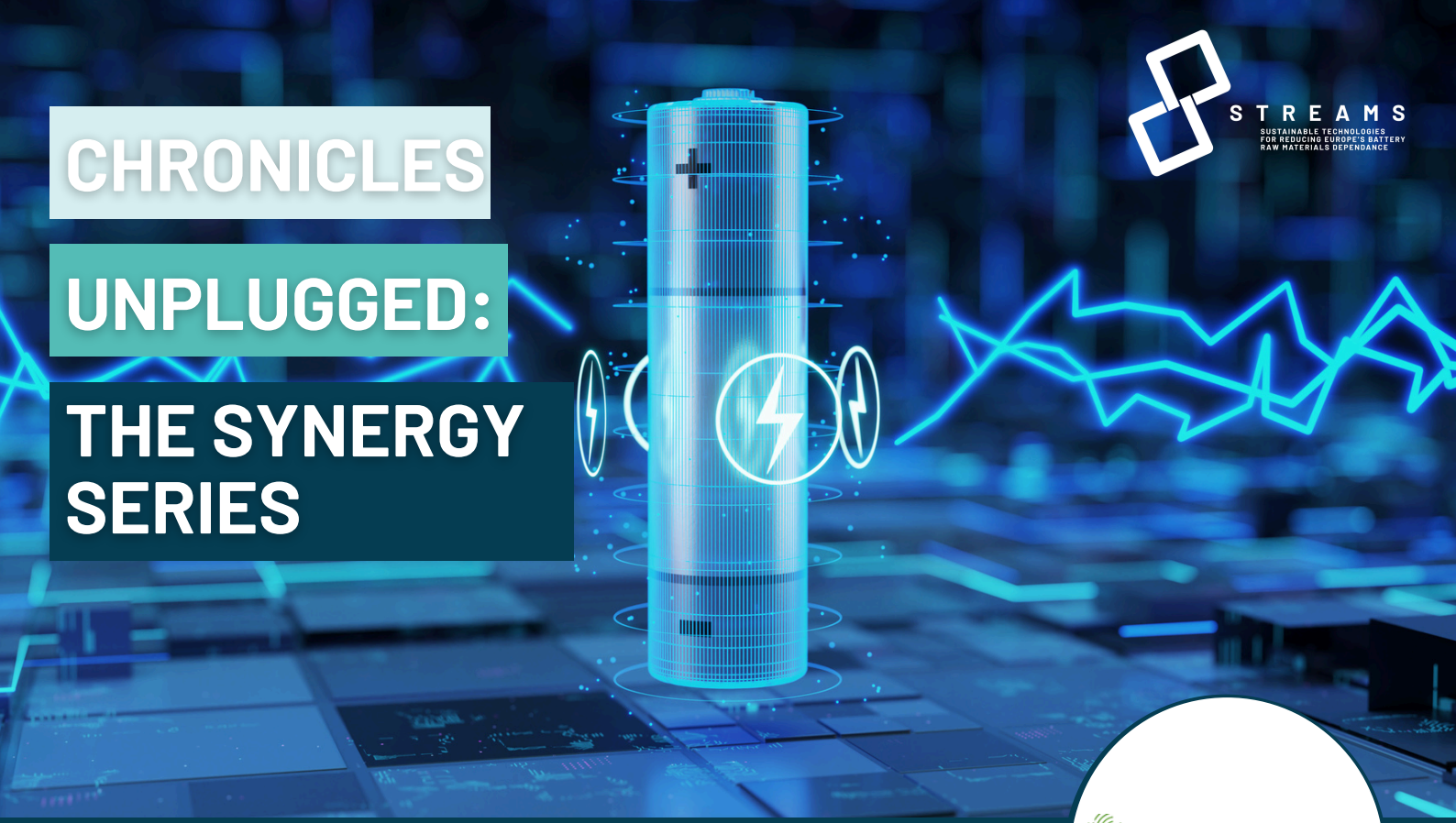

CHRONICLES UNPLUGGED: THE SYNERGY SERIES

STREAMS
SUSTAINABLE TECHNOLOGIES FOR REDUCING EUROPE'S BATTERY RAW MATERIALS DEPENDANCE

FULL-MAP

FULL-MAP

Bridging the data gap: How Transfer Learning accelerates the shift to new battery materials and chemistries

What if new battery technologies didn't have to start from scratch? In FULL-MAP, Transfer Learning allows researchers to reuse knowledge from data-rich battery chemistries to accelerate the development of safer, cheaper, and more sustainable alternatives, reducing both time and testing requirements.

As the global transition to renewable energy accelerates, the pressure to develop safer, cheaper, and more efficient batteries has never been higher. However, moving from established chemistries such as Lithium Cobalt Oxide (LCO) to newer alternatives like Lithium Iron Phosphate (LFP) often feels like starting all over again because we cannot easily leverage on the experimental data and numerical models that we have collected over decades. By applying Machine Learning-based Reduced Order Models (ML-ROM) and Transfer Learning (TL), we will be able to transfer knowledge from data-rich environments to data-scarce ones, effectively speeding up the innovation in the battery industry.

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The challenge of accelerating battery innovation isn't new, and the scientific community has been actively exploring various avenues. For instance, traditional machine learning models have shown promise in predicting battery performance and lifespan for specific chemistries like LCO and even LFP, leveraging large datasets. However, these models often require retraining from scratch when moving to a new material or chemistry, making the process time-consuming and data-intensive. Our focus with ML-ROM and Transfer Learning aims to directly address this 'cold start' problem, building on existing knowledge rather than always starting anew.

The data dilemma: We can't wait for decades of testing

In the world of battery research, data is most valuable. For decades, LCO has been one of the most common chemistries for Lithium-Ion Batteries, resulting in decades worth of experimental and numerical data regarding its thermal behaviour, degradation patterns, and electrochemical performance. In contrast,LFP has very recently come to the fore, mainly due to its safety and cost-effectiveness. However, as it only surged recently, our library of LFP-related data is significantly smaller than other materials and chemistries.

Indeed, traditionally, developing a new battery chemistry requires thousands of hours of physical cycling and dedicated tests. For this, we cannot rely solely on physical testing, as the time-to-market for new LFP-based innovations could take years. This is where physics-based simulation comes in. High-fidelity models can simulate battery behaviour, capturing all the underlying physics. However, they are computationally expensive, often taking hours or days to simulate only a short time interval.

To solve this, we need to use **Reduced Order Models (ROM)**. A ROM is essentially a simplified model that keeps the high-fidelity physics but reduces the computational expense. Within our current research framework, specifically in the activities led by Siemens Digital Industries Software (SISW) and supported by partners Ikerlan and Vrije Universiteit Brussel (VUB), we are using Machine Learning (ML) to build these ROMs. Nevertheless, there is a catch: the training stage for these ML models is very data intensive. An important problem remains: How do we train an ML-ROM to predict LFP battery behaviour accurately if we don't have enough data for LFP to build an accurate ROM? This is where Transfer Learning comes in.

Transfer Learning: Teaching an old model new tricks

The answer lies in **Transfer Learning (TL)**, the main theme that is covered in **Task 2.5 of FULL-MAP**. You can think of Transfer Learning as follows; a student who through years of study has mastered Italian and is now trying to learn Spanish. Because, through their knowledge of Italian, they understand the underlying structure of Romance languages, they don't need to start from scratch; they simply need to enrich their Romance language base with the specific differences in vocabulary and grammar that the Spanish language brings. In our analogy, the "Italian" is the wealth of data we have for LCO, and the "Spanish" is the emerging data for LFP.

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A Transfer Learning process breaks down into two key steps:

Step 1: Learning from heterogeneous data

First, we **develop a robust ML-ROM based on the available set of heterogeneous data**, supported by WP 1 which is responsible for the Data specification, collection, analysis and management. This data, which **often has different origins** includes data from laboratory experiments (WP 4 – Advanced characterisation and testing) , high-fidelity physics models (WP 3 – Multi-scale and multi-physics simulations and modelling at material, component and cell level), historical datasets, etc. By combining these, the ML model learns the fundamental laws of physics describing battery behaviour: how ions move, how heat is generated, how materials expand and contract, etc. At this stage the model in our example might be heavily weighted toward LCO characteristics, but it will also have developed a deep understanding of battery physics.

Step 2: Transferring knowledge

Once the base model is trained, we **apply Transfer Learning to adapt it to the new material and/or chemistry**, in our example LFP. Instead of training a new ML-ROM from zero, we freeze the layers of the neural network that understand the general physics and only retrain the final layers that are specific to the material/chemistry with the limited LFP data available.

Within the FULL-MAP project, we focus our Transfer Learning on two application cases:

- **Accelerate materials screening**: Using computational chemistry tools originating from Task 3.1 (Active materials design) we can test thousands of material variations in silico without ever stepping into a lab. Instead of requiring a massive, independent dataset for every new iteration, Transfer Learning allows us to leverage the general physics learned from data-rich chemistries (such as e.g. LCO) and enrich it with dedicated simulations on a new data-poor chemistry (e.g. LFP). This enables us to predict critical properties like ion diffusion and conductivity with far less effort, effectively reducing the time required to screen new materials by building upon established expertise.

- **Predict battery cell KPIs**: By transferring the Key Performance Indicators (KPIs) and the physics of battery ageing learned from decades of LCO data, we can accurately predict the behavior of newer LFP cells, leveraging on Task 3.6 developments where we develop high-fidelity models of the battery cell performance and degradation like lithium plating and particle cracking.

Furthermore, Transfer Learning can and will be deployed much more broadly in the future in cases where we are facing the cold start problem, having little-to-no data for emerging technologies.

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From theory to integration: The FULL-MAP Orchestrator

A breakthrough in the lab is only useful if it can be used by the industry. One of the most exciting aspects of our work is how we are ensuring these models are accessible to manufacturers, OEMs, and the wider scientific community through the **FULL-MAP platform**.

We envision this platform as an **agent orchestrator** situated at the intersection of language models, reasoning systems, and foundation models. Rather than relying on isolated software silos, this orchestrator coordinates a library of pretrained, domain-specific models and integrates them directly into research and production workflows. By using a capable reasoning framework to select and adapt existing models to perform previously missing prediction steps within the workflow, we ensure compatibility across the entire battery value chain, from materials to manufacturing to application. This allows the knowledge transferred from LCO to LFP to flow freely, enabling users to adapt their strategies to new chemistries quickly.

Looking ahead: A faster path to sustainability

The work we are doing in Transfer Learning is **about more than just saving time; it is about making the battery development process more resilient**. By learning how to transfer knowledge between chemistries, we are taking important steps to bring new materials, such as solid-state electrolytes or sodium-ion batteries, much faster to the market.

The Transfer Learning **activities have recently started at project partners SISW, Ikerlan and VUB**. The insights we are gaining from these material screenings and virtual performance testing will help the industry move faster toward new chemistry options, providing a roadmap for how ML-ROMs can be exploited by the orchestrator.
In the FULL-MAP project we are refining these models and pushing the boundaries of what is possible in battery testing and simulation. The transition to a sustainable, electrified future depends on our ability to innovate faster than ever before, and with Transfer Learning, we are doing exactly that.

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