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# Accelerated Thermal Battery Design Through Digital Engineering Tools

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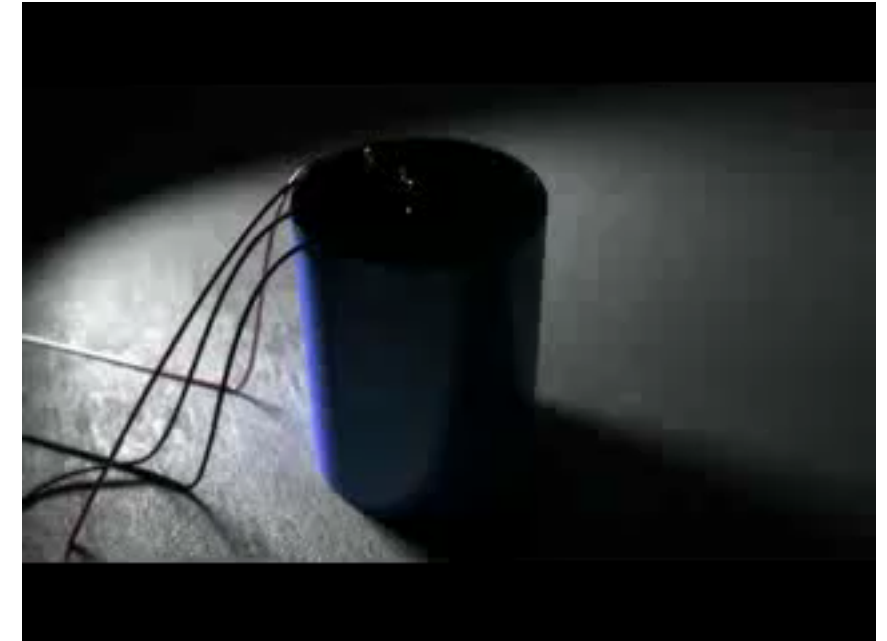
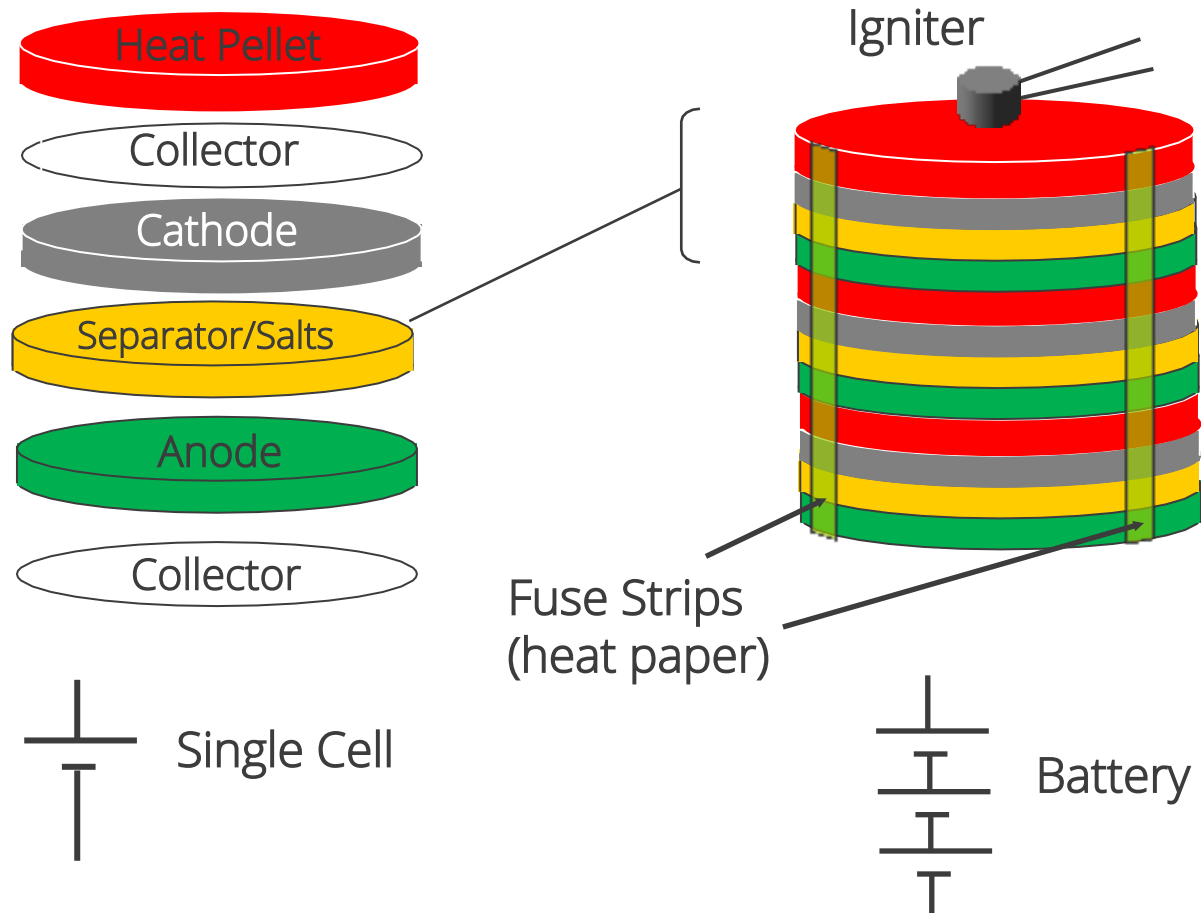
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Sponsors: Advanced Simulation and Computing (ASC) P&EM and V&V elements, ADE initiative



# What is a thermal battery?



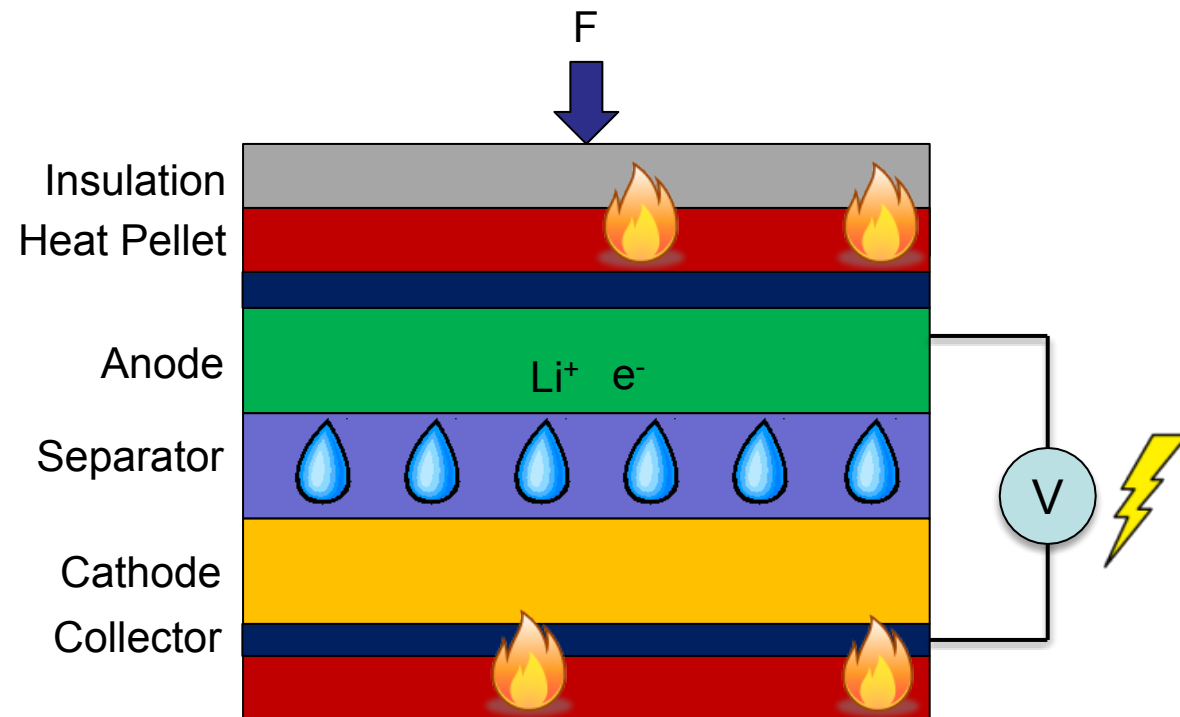
Thermal batteries provide high power density, high reliability, and a long shelf life.



# What makes a thermal battery work?

Battery activation is a complicated, multi-step process

- Heat pellet burning
- Thermal diffusion
- Melting and flow of the electrolyte
- Deformation of the separator
- Rebound of the insulation
- Activation

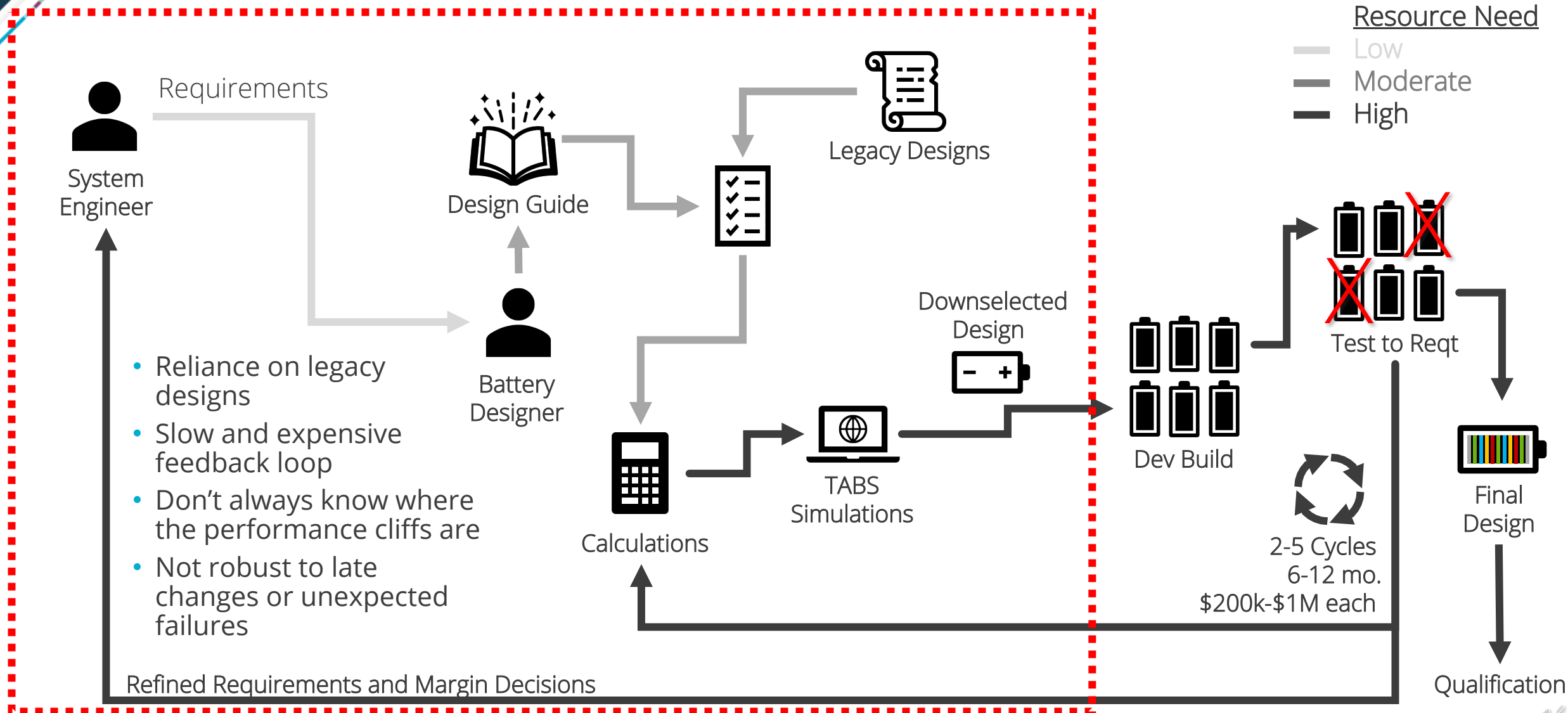


Thermal battery activation is a true multi-physics process!





# Current state of thermal battery design

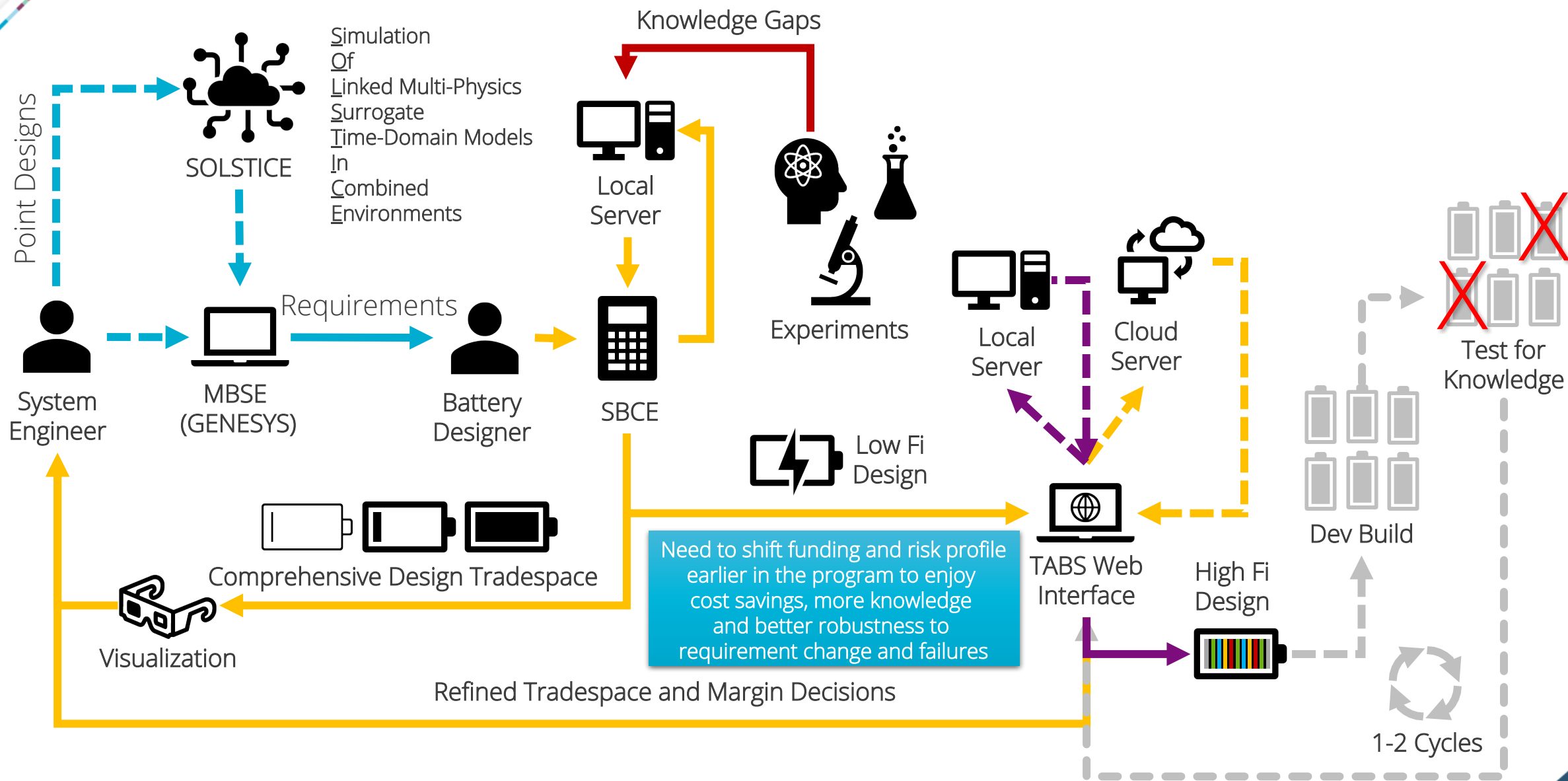


Current battery design process is nowhere near optimal





# Vision for accelerated digital engineering of batteries

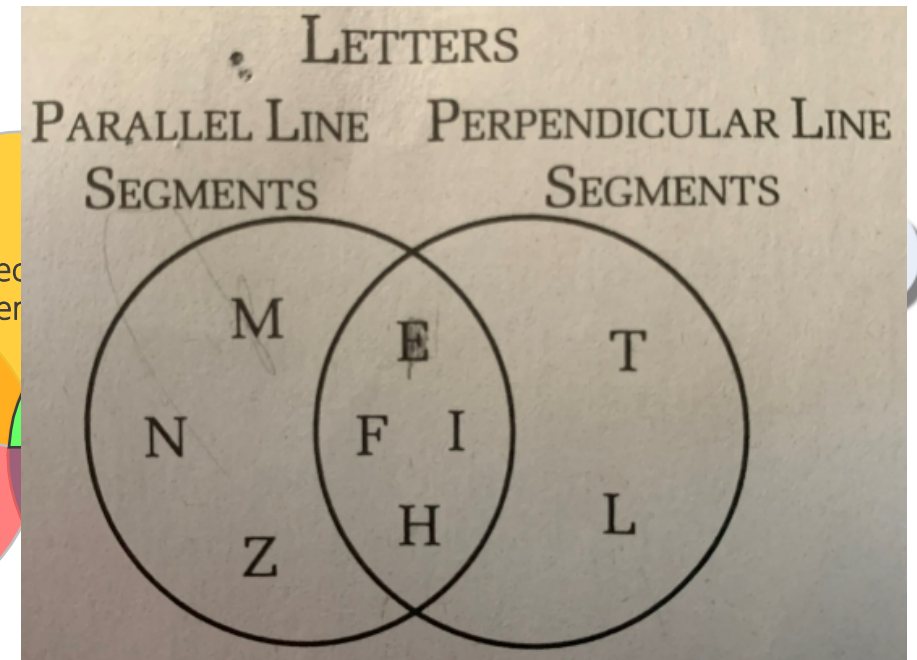
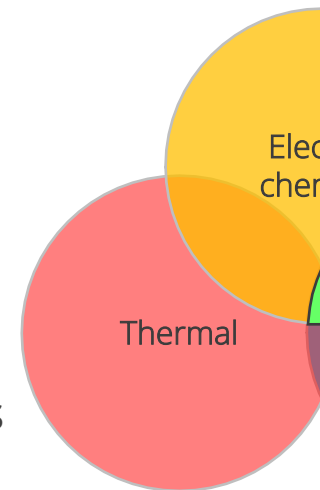




# Set-Based Concurrent Engineering

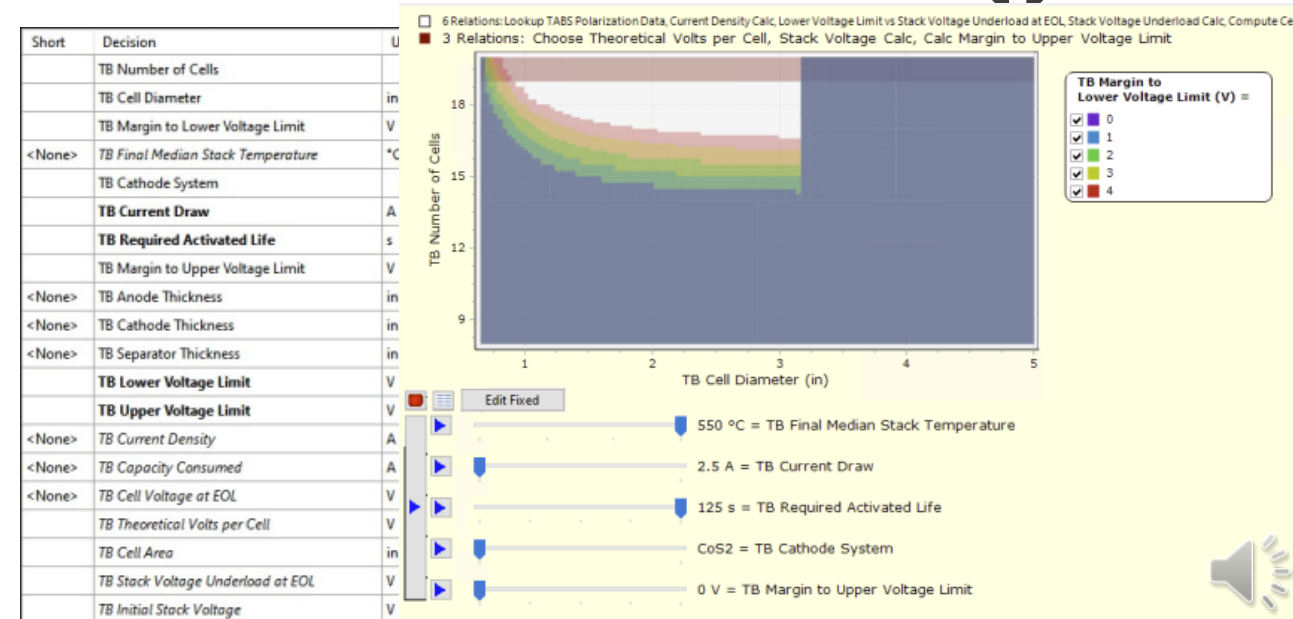
What is SBCE?

- Set-Based: Finding the set of all feasible solutions given all requirements and constraints
- Concurrent: Convergence of the set of system solutions occurs simultaneously with convergence of the set of subsystem or component solutions
- Thermal Battery team uses software called Success Assured



How does it work?

- Building blocks
  - Requirements, Design Choices, Relations
- Tools
  - Causal Maps (knowledge gaps)
  - Solvers (compatibility)
  - Limit Charts (feasible design space)
- Goals
  - gaining knowledge
  - finding compatible ranges for design variables
  - defining the set of all feasible designs

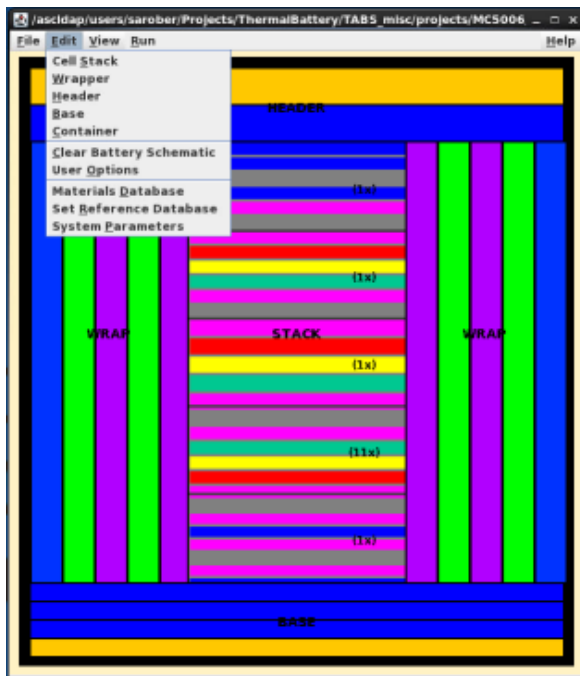




# TABS: The Thermally Activated Battery Simulator

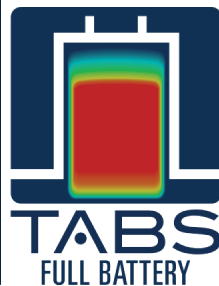
## TABS design principles

- Create a user interface **intuitive to battery designers**, not just for computational scientists
- Be **computationally efficient**, so many design iterations can be explored in a single work day
- Present the user with the most **relevant quantities of interest**, yet enable them to explore more deeply
- Have **demonstrated credibility**, such that the user knows when and how much to trust the solutions



## TABS-FB: Full Battery

- Thermal
- WIP: Electrochemical



## TABS thermal realized impacts

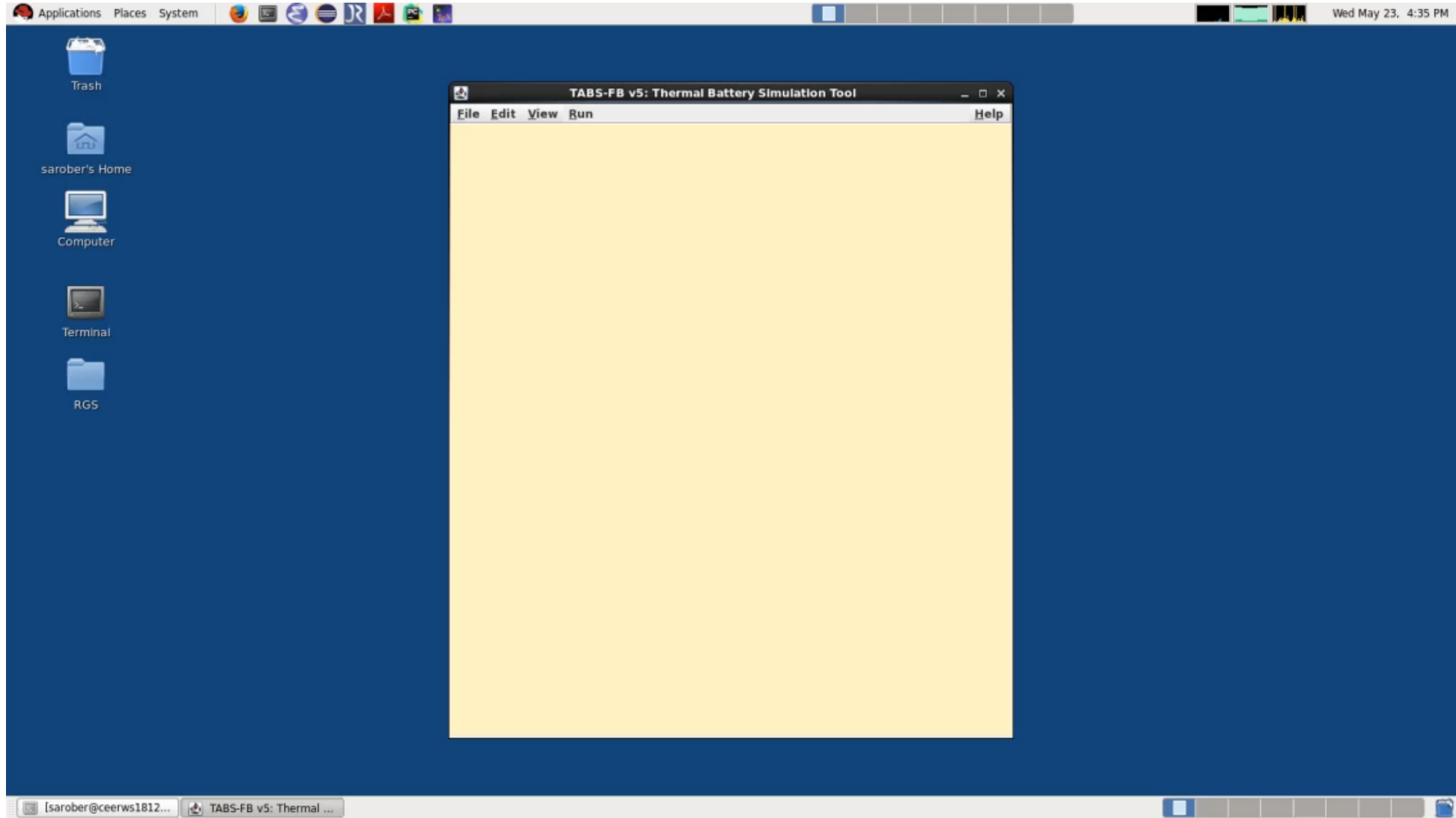
- Saved \$3.6M and 13 months of schedule on two recent life extension programs
- Cost savings recouped ASC investments to date
- Enabled first fully virtual battery design for external customer
- Yielded insight into anomalous test behavior

TABS provides battery designers the power to understand how design decisions impact performance





# Thermal design analysis in 5 minutes using TABS







## So what's wrong with TABS?



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Legacy TABS is powerful and impactful, but not prepared to maximize potential





# Full battery electrochemical simulations

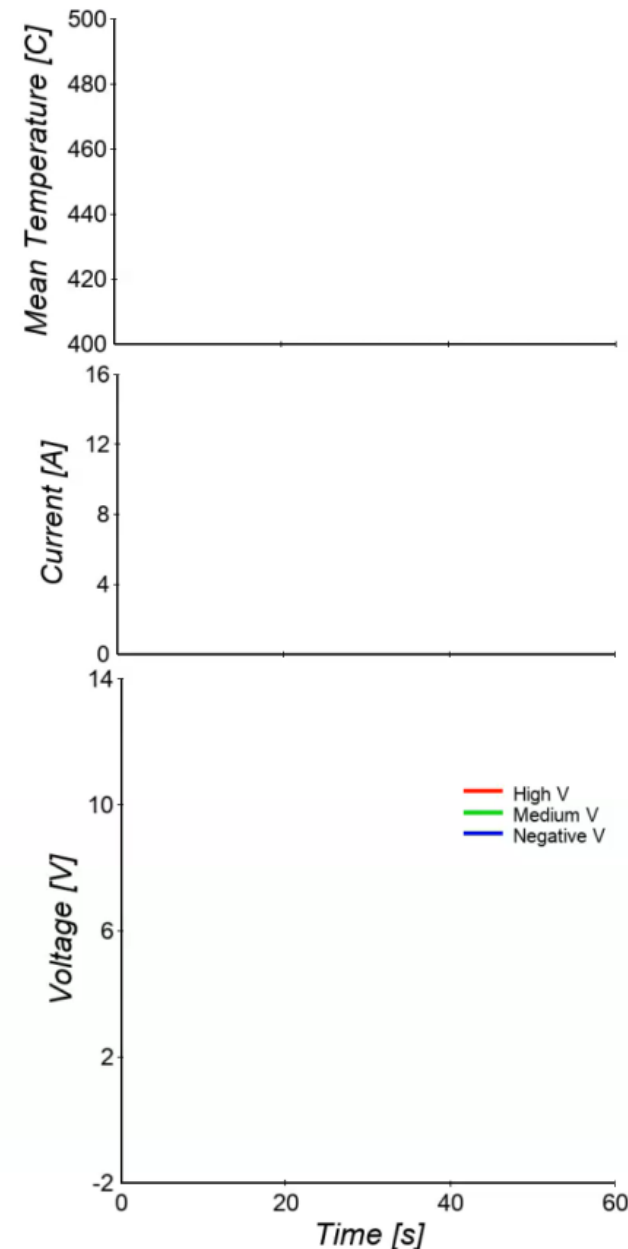
Time = 0.00 s

Current Density [A/m<sup>2</sup>]  
0.0e+00 5.0e+04 1.0e+05



Temperature [C]  
0 150 300 450 600

Voltage [V]  
-2 2 6 10 14  
0 4 8 12





# Making TABS a web-based productivity tool for battery designers

The collage shows the following screenshots of the TABS application:

- Welcome to TABS:** The main landing page with options to create a new battery or import an existing one. It includes a 'Blank Battery' section and a 'Battery Templates' section.
- Battery Workflow:** A sidebar menu with options like Project Details, Design & Material Specifications, Environment, Summary/Preflight Check, Simulation Parameters, and View Results.
- Electrochemical Boundary Conditions:** A section for defining battery parameters, including a 'Full Battery' configuration with a diagram of a battery cell.
- Summary/Preflight Check:** A section for reviewing battery statistics, including Size (3.3 x 5.2 Feet), Weight (12 pounds), Diameter (12 inches), Volume (100 liters), Heat Balance (12 kcal), Current (300000 volts), and Nominal Voltage (12V).
- View Results:** A section for viewing simulation results, including a '2D Plots' section with a 'Tracer History' plot and a 'Performance Metrics' section showing various temperature and voltage metrics.

The application interface is designed to be user-friendly and intuitive, with clear navigation and detailed data visualization.

UX research teaches us how battery engineers want to interact with TABS



# Making TABS a productivity tool for battery designers

The screenshot shows the 'Inside' web application at `inside.sandia.gov`. The interface includes a top navigation bar with links for 'Directory', 'Policy', and 'News', and a search bar for 'People/Orgs'. A secondary bar shows the current location as 'Albuquerque' at '49°F' and a 'What's New' section with a user profile for 'Scott Roberts'. The main content area is divided into several sections: 'Tools to get work done' with buttons for 'Most Used' and 'By Category'; a row of featured announcements including 'WebShipper2.0 down noon 2/25', 'Office 365 Training', 'Delve & File Sharing in O365', 'ASC S<sup>3</sup>C call for papers', 'External Thunderbird UI', and 'New! IaC via Terraform'; an 'INDEX' section with an alphabetical list; a 'Feedback' button; a 'Latest coronavirus information/FAQ and update messages' banner; an 'Around Sandia' section featuring a 'Black History Month' announcement with 11 comments; a 'Directory Quick Search' section with a search input and an 'Advanced Search' link; and a 'My Links' section with '+ Add Group' and 'Visit the My Links Tutorial' options.

Web application with HPC-backed computation will provide more capability with easier access



# Fully-Integrated Digital Workflow

