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# Accelerated Thermal Battery Design Through Digital Engineering Tools

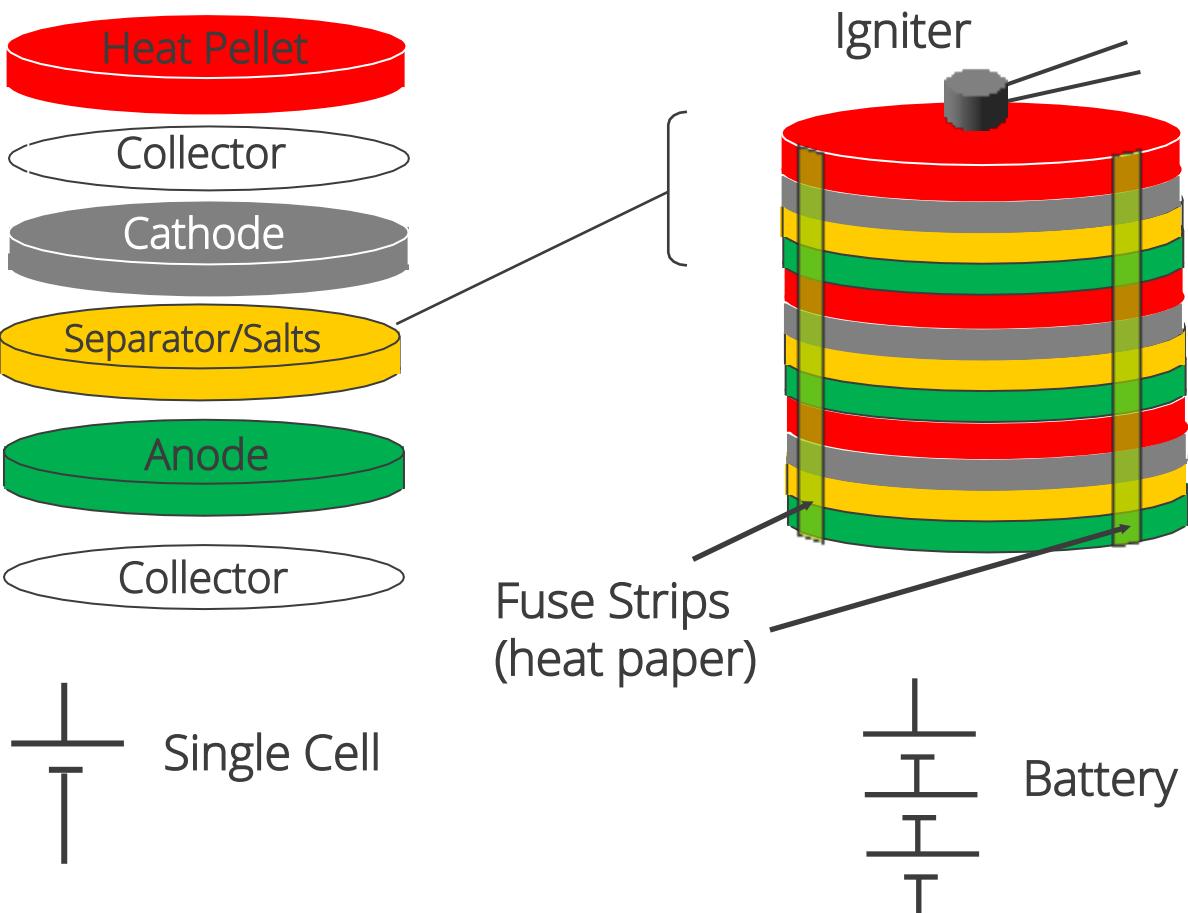
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Sponsors: Advanced Simulation and Computing (ASC) P&EM and V&V elements, ADE initiative

# What is a thermal battery?



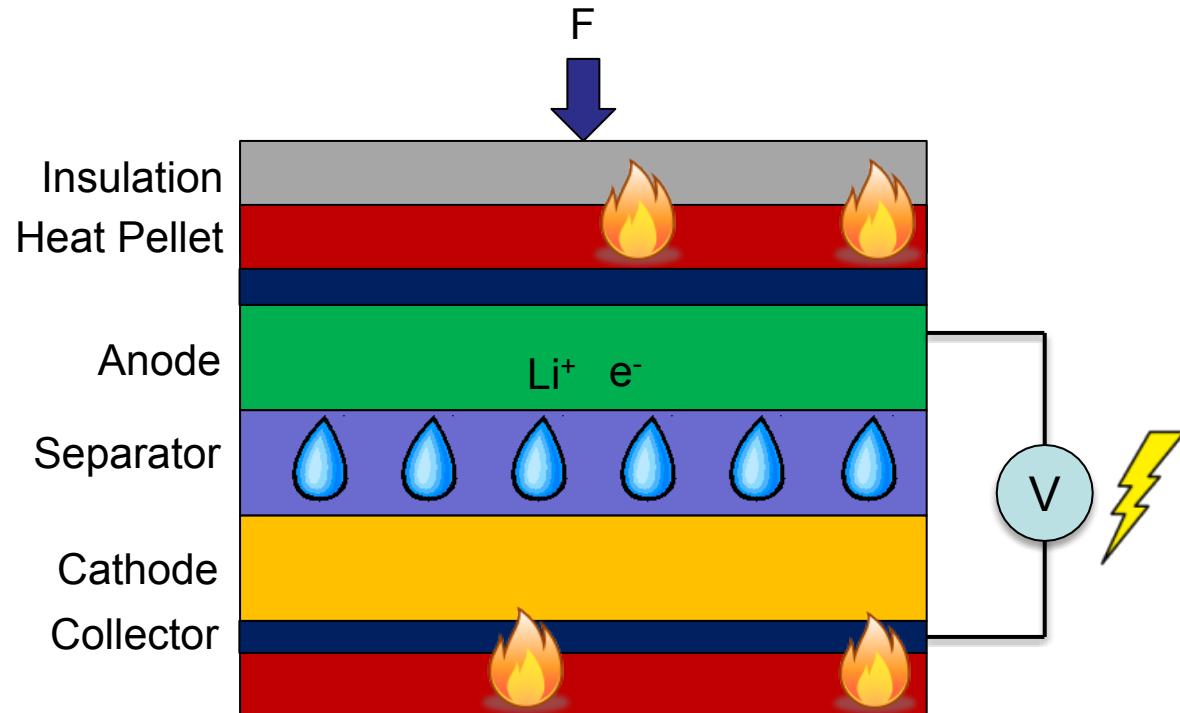
Thermal batteries provide high power density, high reliability, and a long shelf life.



# What makes a thermal battery work?

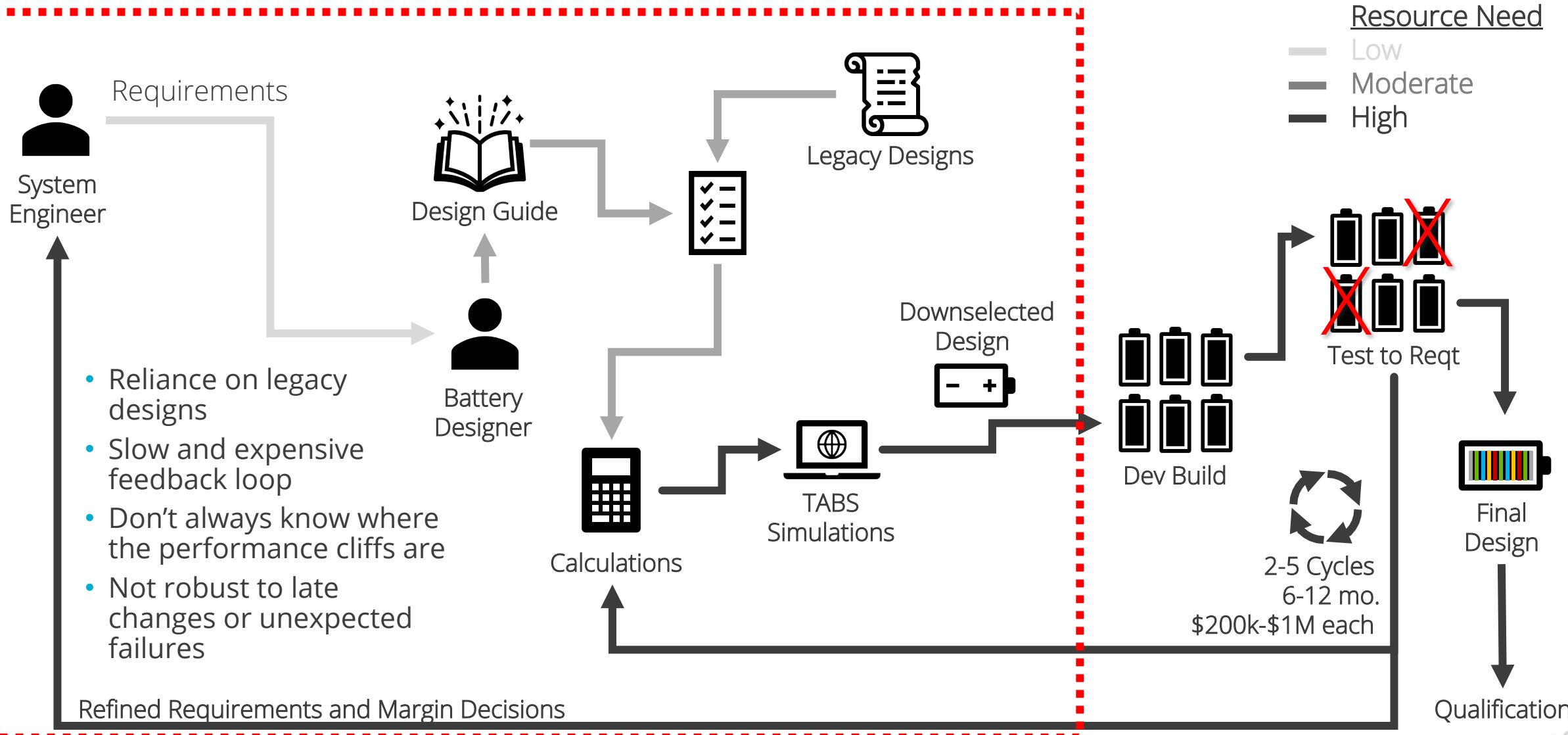
Battery activation is a complicated, multi-step process

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



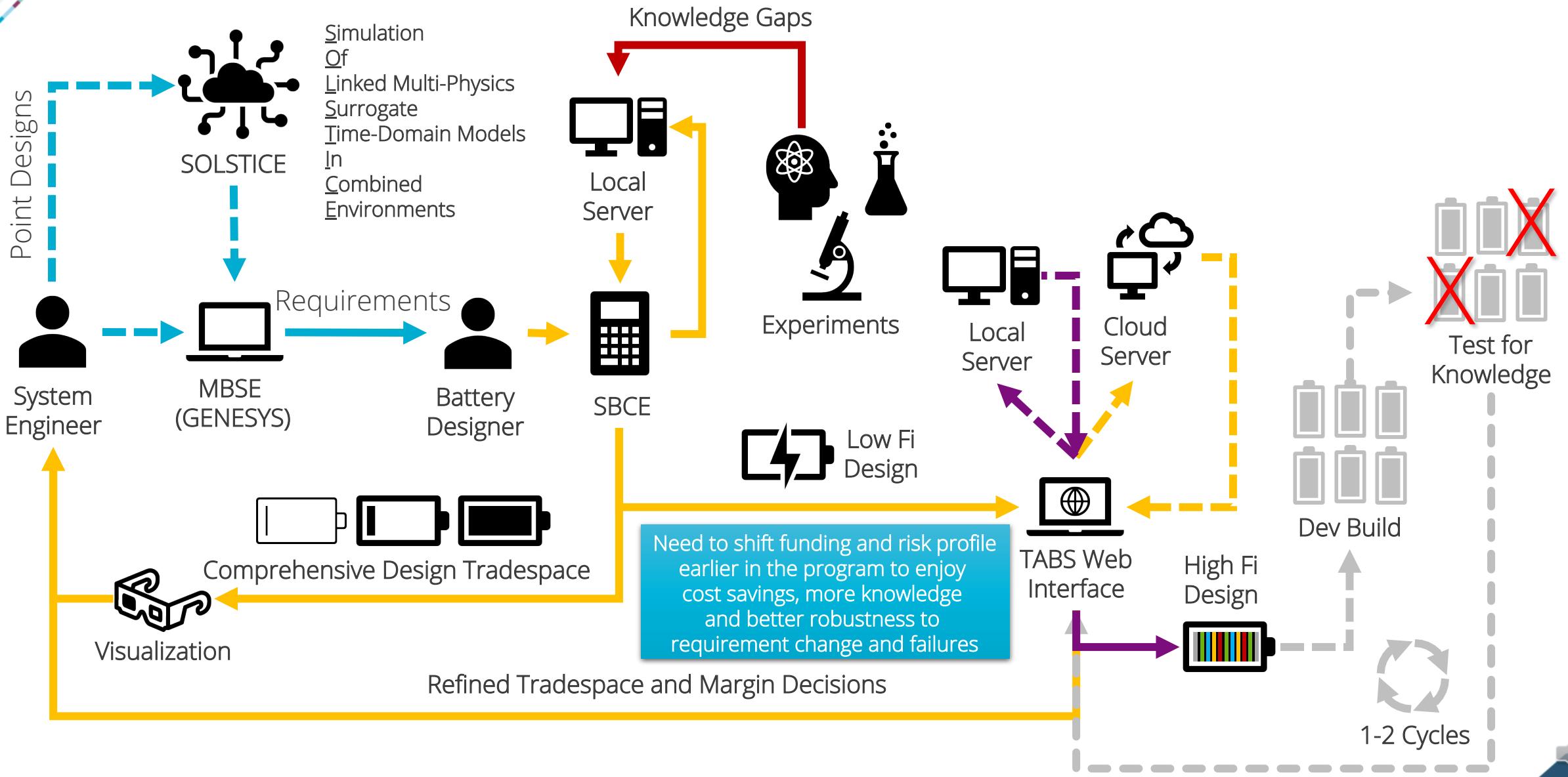
Thermal battery activation is a true multi-physics process!

# Current state of thermal battery design



Current battery design process is nowhere near optimal

# Vision for accelerated digital engineering of batteries





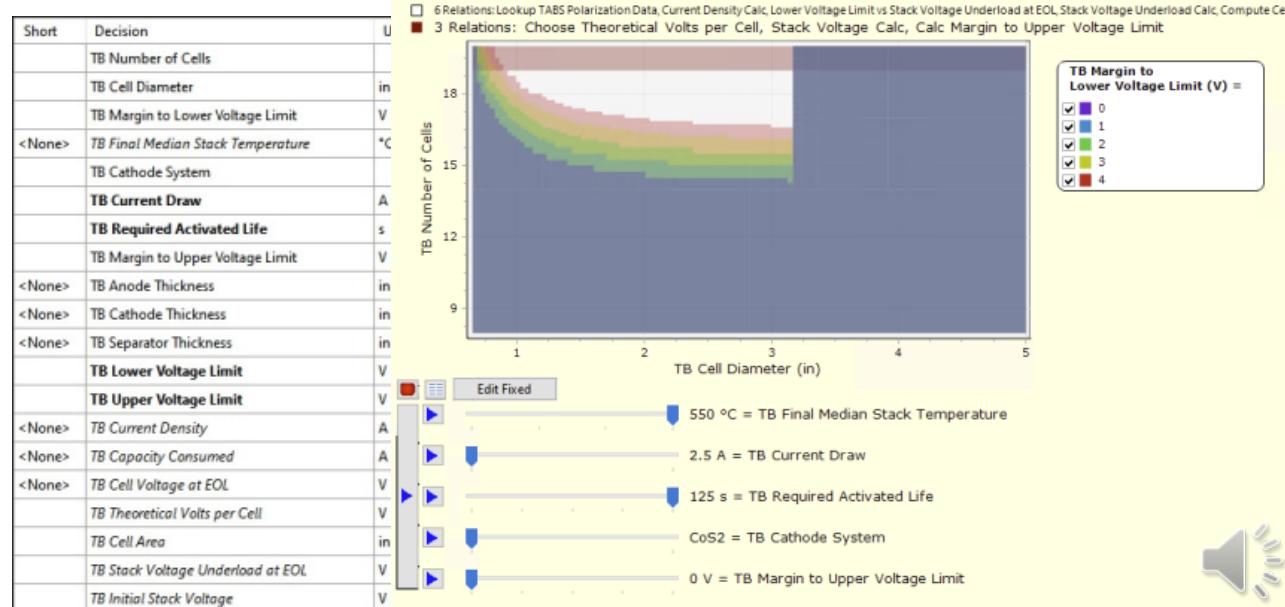
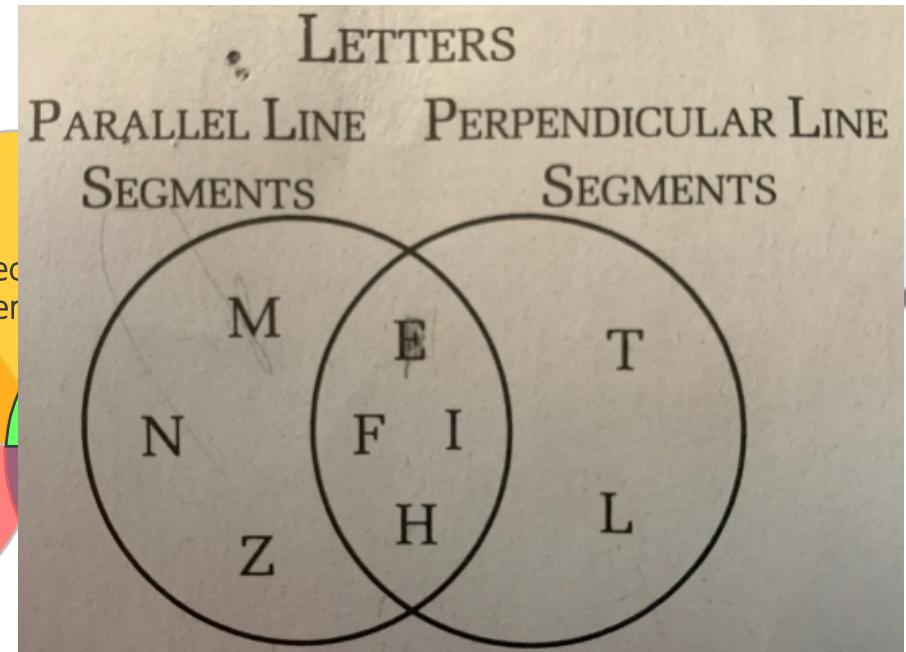
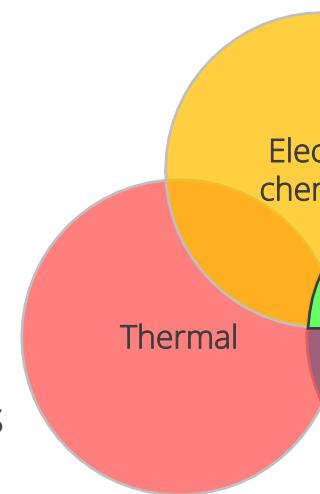
# Set-Based Concurrent Engineering

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

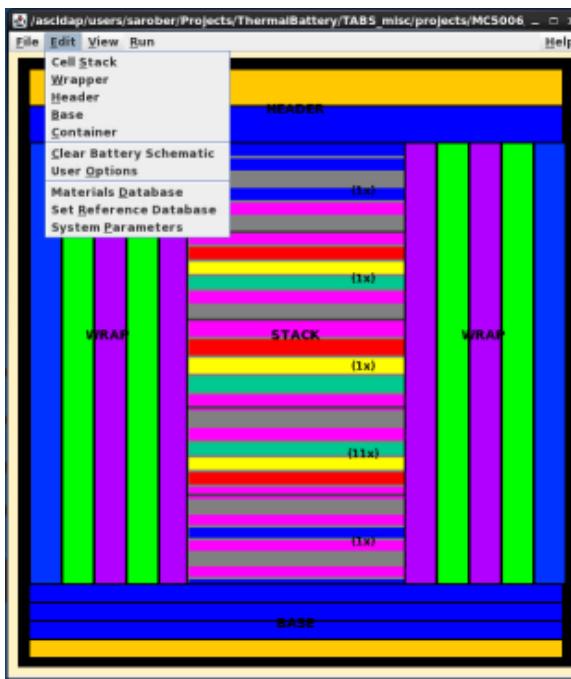




# TABS: The Thermally Activated Battery Simulator

## 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



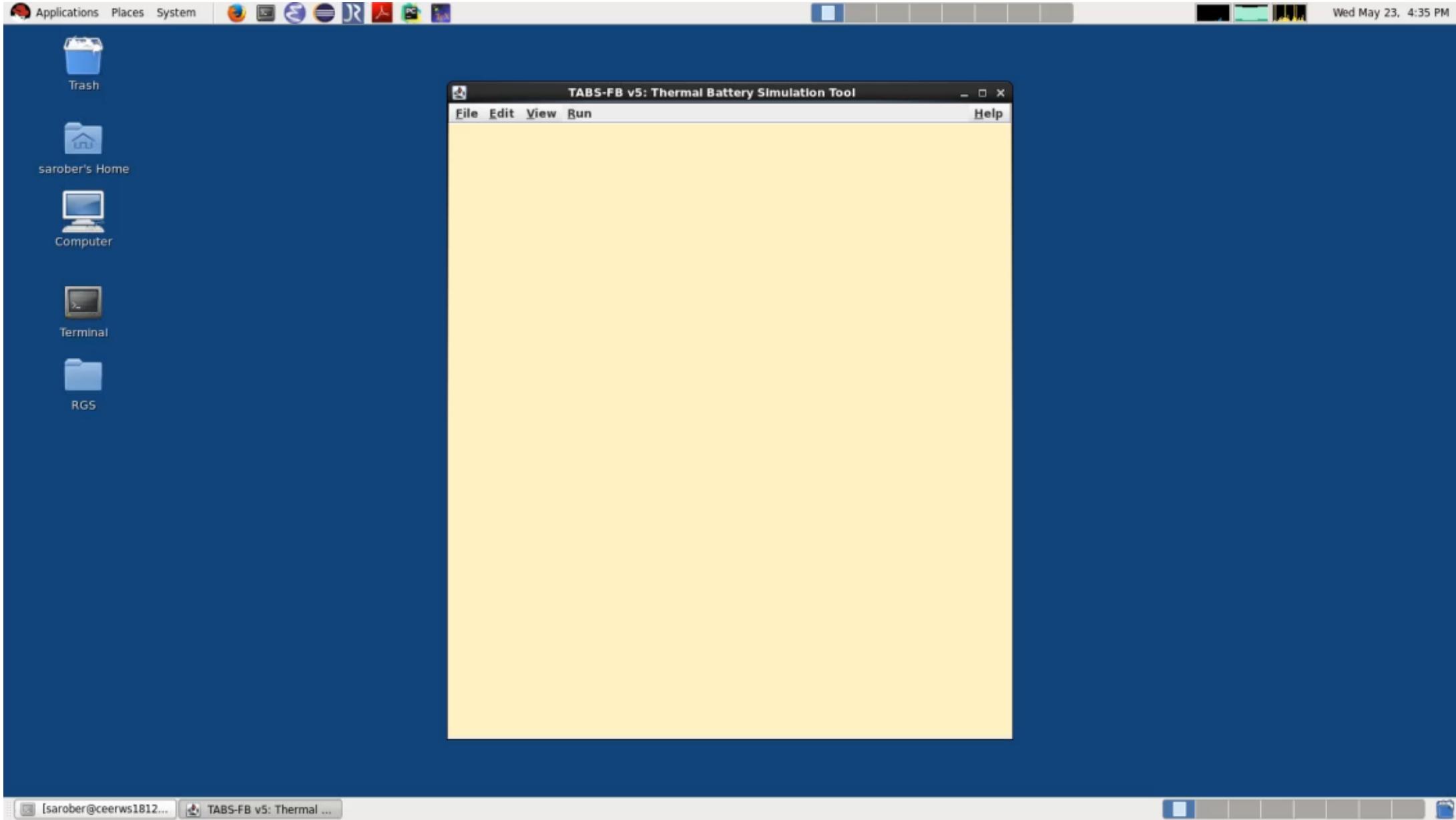
## TABS thermal realized impacts

- 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

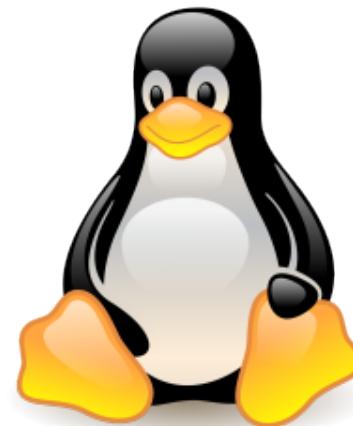


# Thermal design analysis in 5 minutes using TABS





## So what's wrong with TABS?



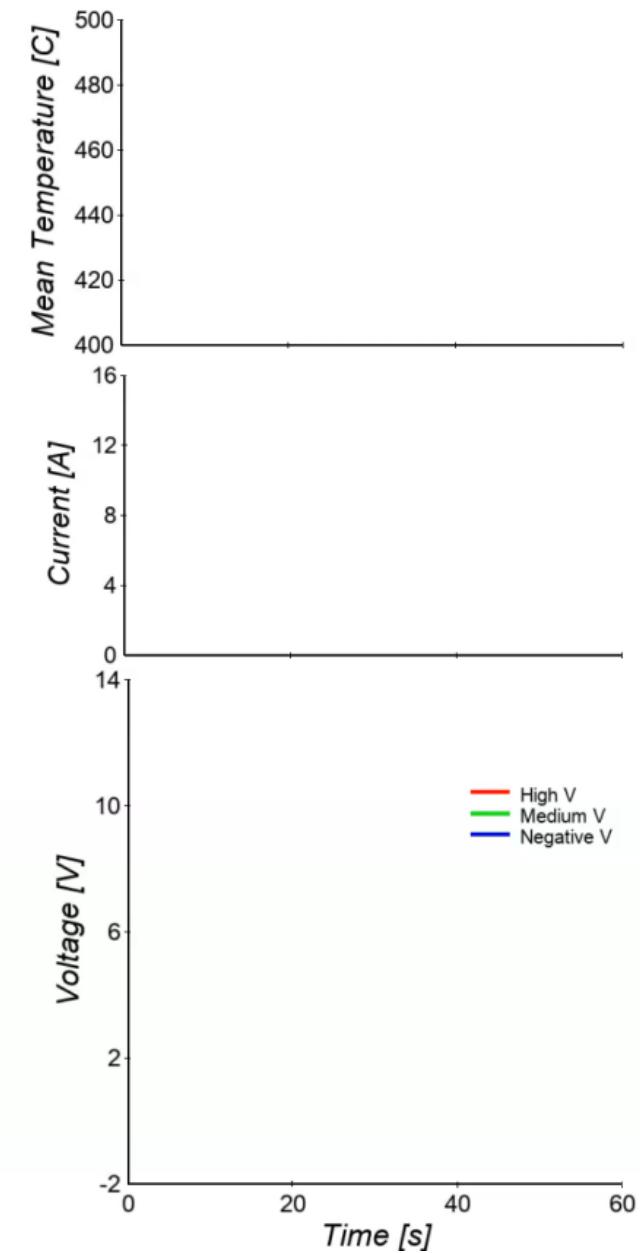
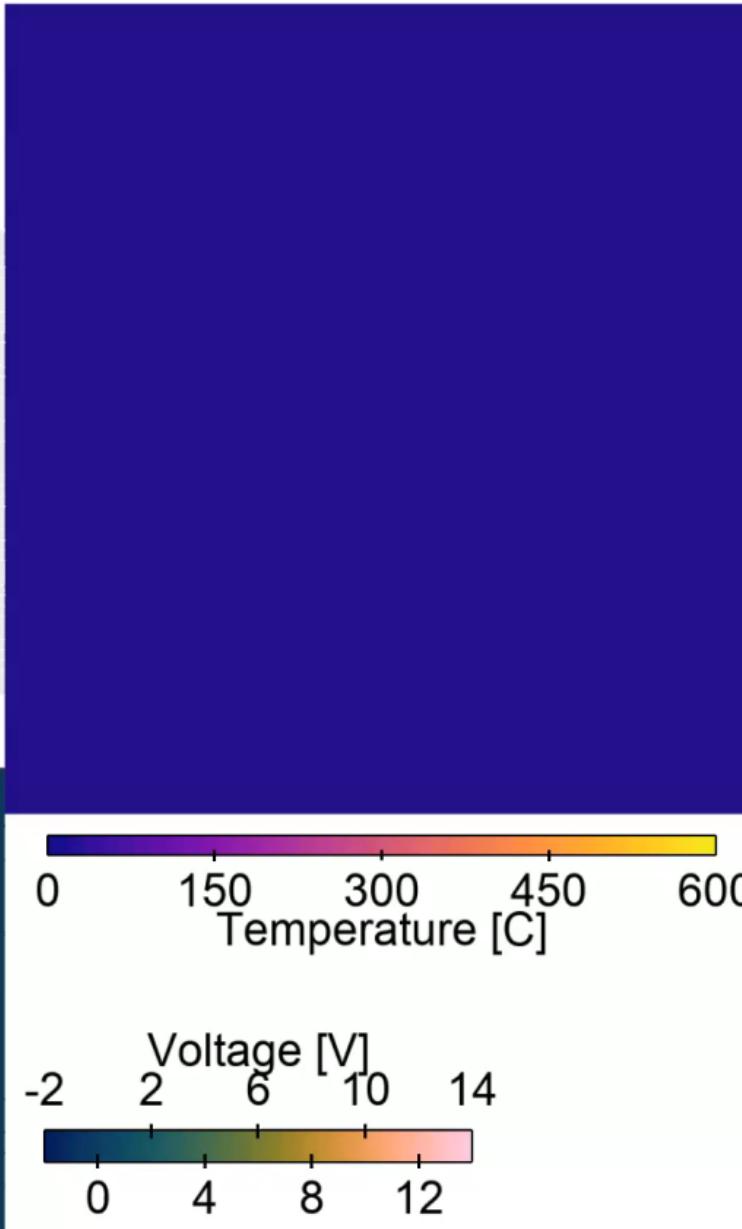
Legacy TABS is powerful and impactful, but not prepared to maximize potential



# Full battery electrochemical simulations

Time = 0.00 s

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





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

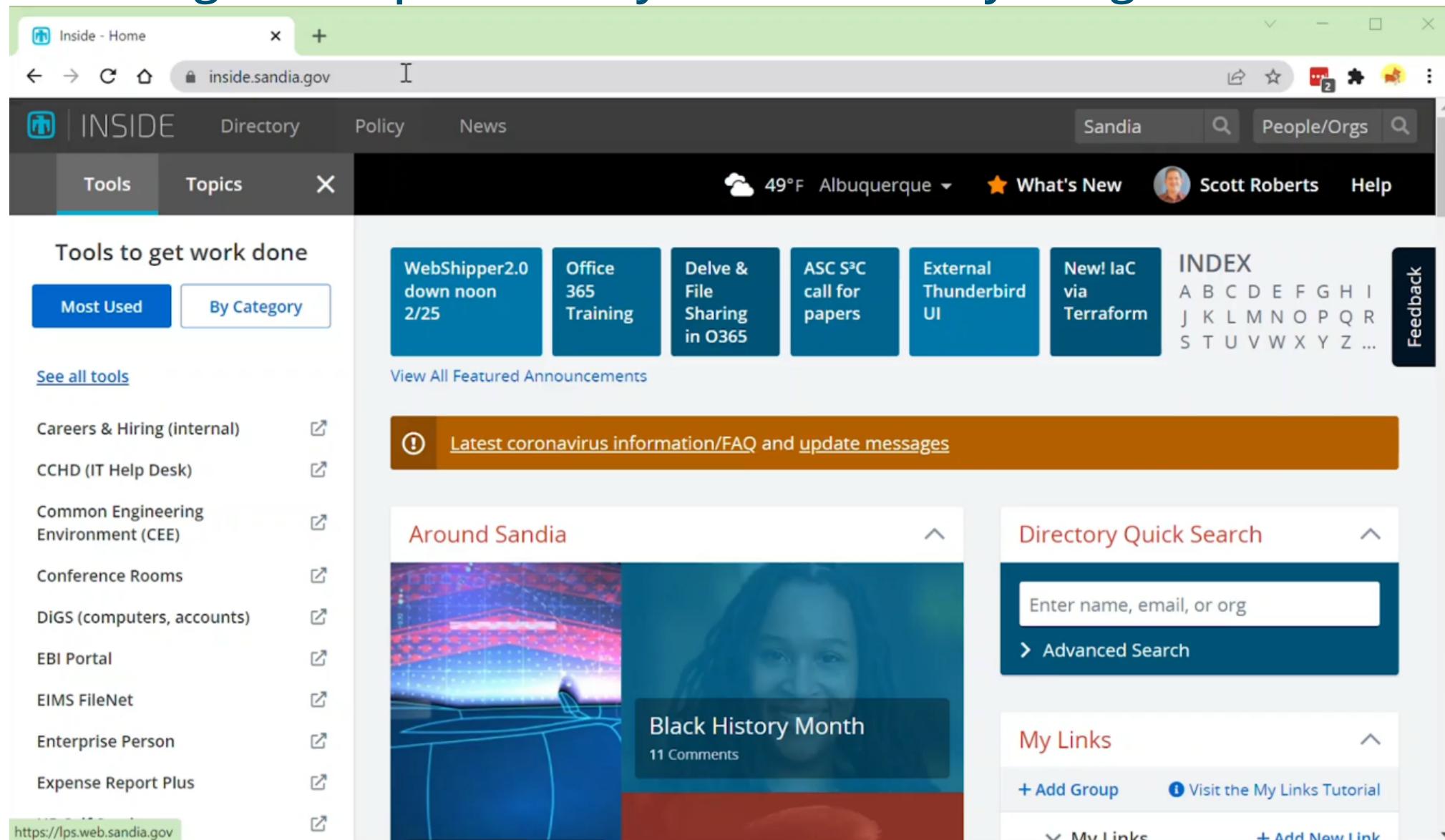
The image displays three side-by-side screenshots of the TABS (Thermally Activated Battery Simulation Tool) software interface, illustrating its features and design.

- Home Screen:** Shows the "Welcome to TABS" page with a "Blank Battery" template, an "Import" option, and a "Battery Templates" section with three icons for different starting points.
- Battery Workflow:** Shows the "Electrochemical Boundary Conditions" and "Battery Scenarios" sections. It includes a 3D model of a battery cell with various components labeled (CASE, HEADER, BASE, ISLAP, STACK, SEPARATOR, ANODE, CATHODE, INSULATION, and VOLTAGE TAPs). The "Battery Statistics" panel provides key data: Size (3.3 x 5.2 feet), Weight (12 pounds), Diameter (12 inches), Volume (100 liters), Heat Balance (12 kcal), Current (3000000 volts), Nominal Voltage (12), and a "Materials Color Legend" and "Thermal BC Legend".
- Results View:** Shows the "View Results" section with a "2D Plots" panel displaying "Tracer History" plots for Temperature (K) vs. Time (seconds) and Current (A) vs. Time (seconds). The "Performance Metrics" panel lists various thermal and electrical parameters, all showing values of 800 degrees Celsius. The "Summary Data" panel shows "Design & Material Specifications" for Group 1: Insulation and Group 2: Cells, listing materials like Separator 1, Anode, Cathode, and Separator 1-2, along with their properties and thicknesses.

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



# Making TABS a productivity tool for battery designers



The screenshot shows the Sandia Inside web application homepage. The top navigation bar includes links for Inside - Home, Directory, Policy, News, Sandia, People/Orgs, and a search bar. The header also displays the location inside.sandia.gov, the weather (49°F in Albuquerque), a 'What's New' section, and a user profile for Scott Roberts. The main content area features a sidebar titled 'Tools to get work done' with 'Most Used' and 'By Category' buttons, and a 'See all tools' link. The main content area displays several featured announcements: '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'. A 'View All Featured Announcements' link is also present. A prominent orange banner at the top of the main content area contains an exclamation icon and the text 'Latest coronavirus information/FAQ and update messages'. Below this, there are two cards: 'Around Sandia' showing a 3D visualization of a battery cell and a woman's face, and 'Black History Month' with 11 comments. To the right, there are search and link management sections for 'Directory Quick Search' and 'My Links'.

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



# Fully-Integrated Digital Workflow

