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Accelerated Thermal Battery Design Through Digital Engineering Tools

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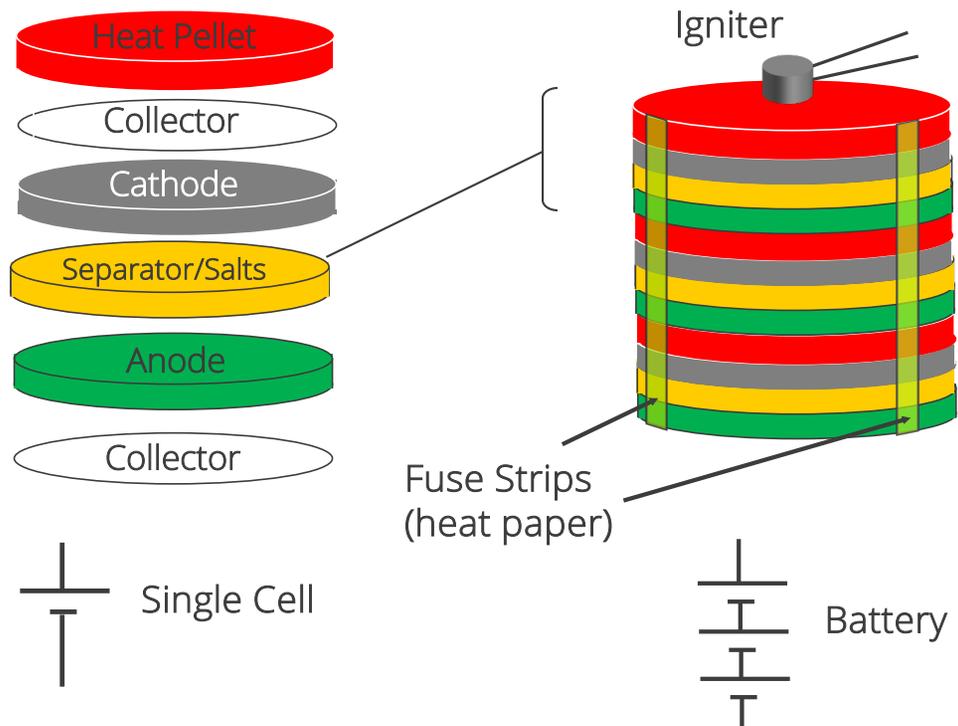
Co-authors: Henry Padilla, Ian Barney; Project Manager: Scott Hutchinson
Sponsors: Advanced Simulation and Computing (ASC) P&EM and V&V elements, ADE initiative

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What is a thermal battery?



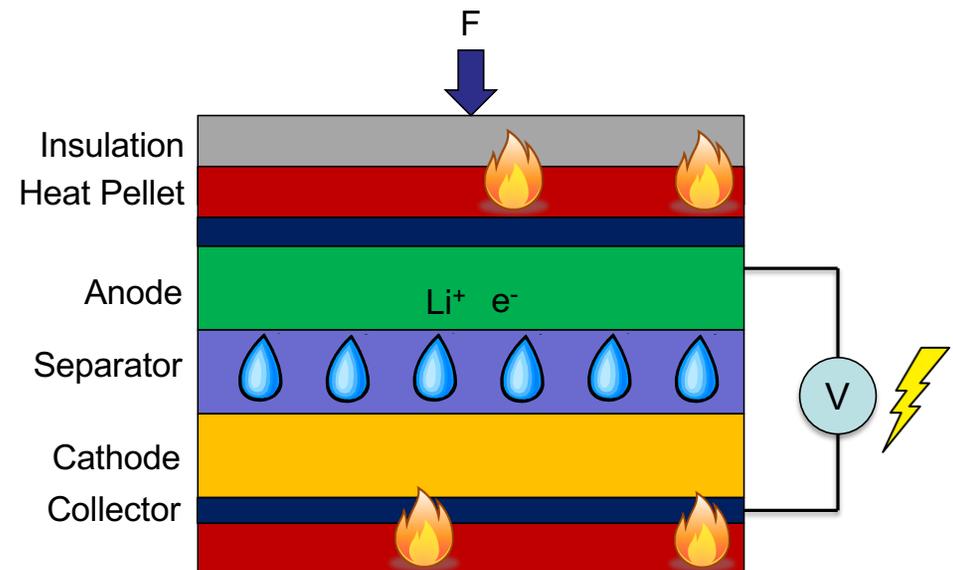
Thermal batteries provide high power density, high reliability, and a long shelf life.



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

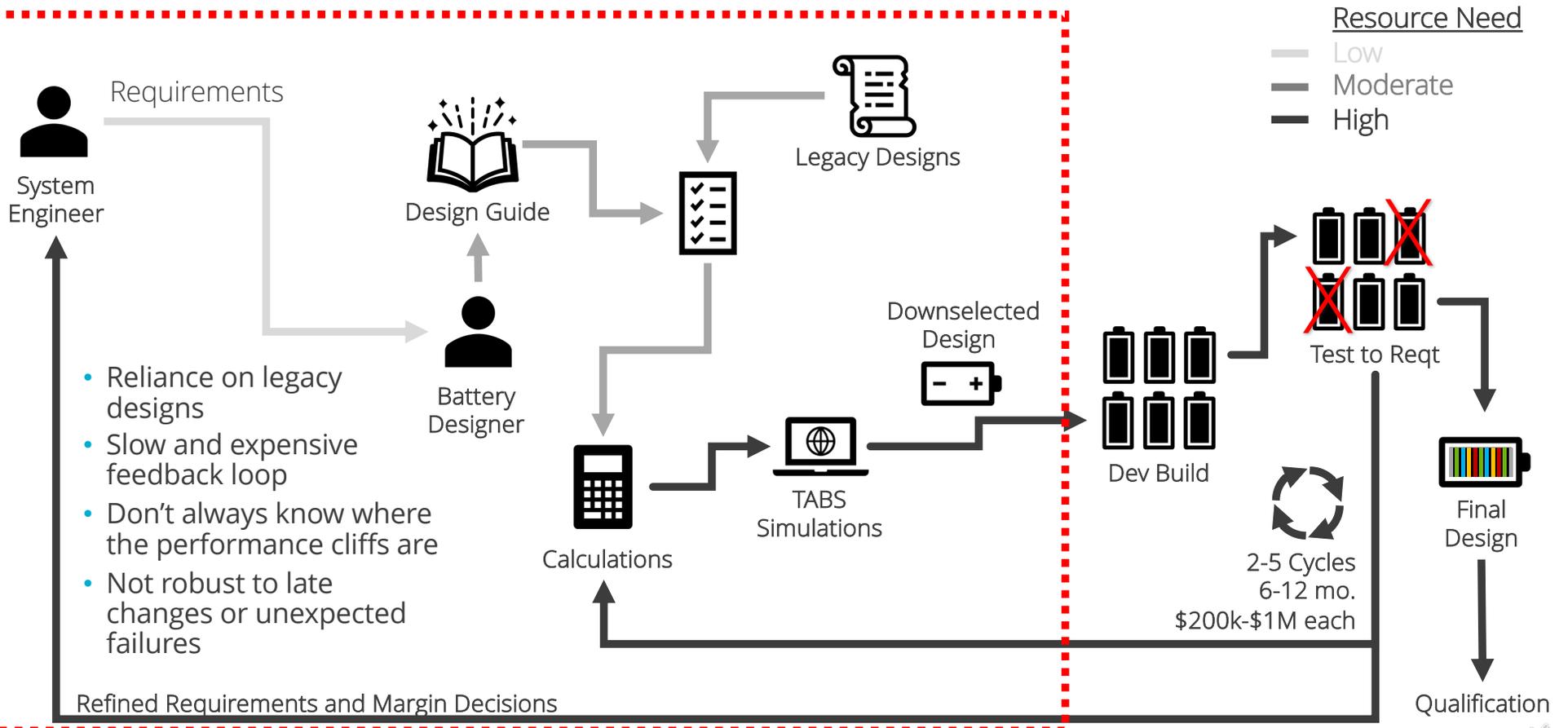


Thermal battery activation is a true multi-physics process!





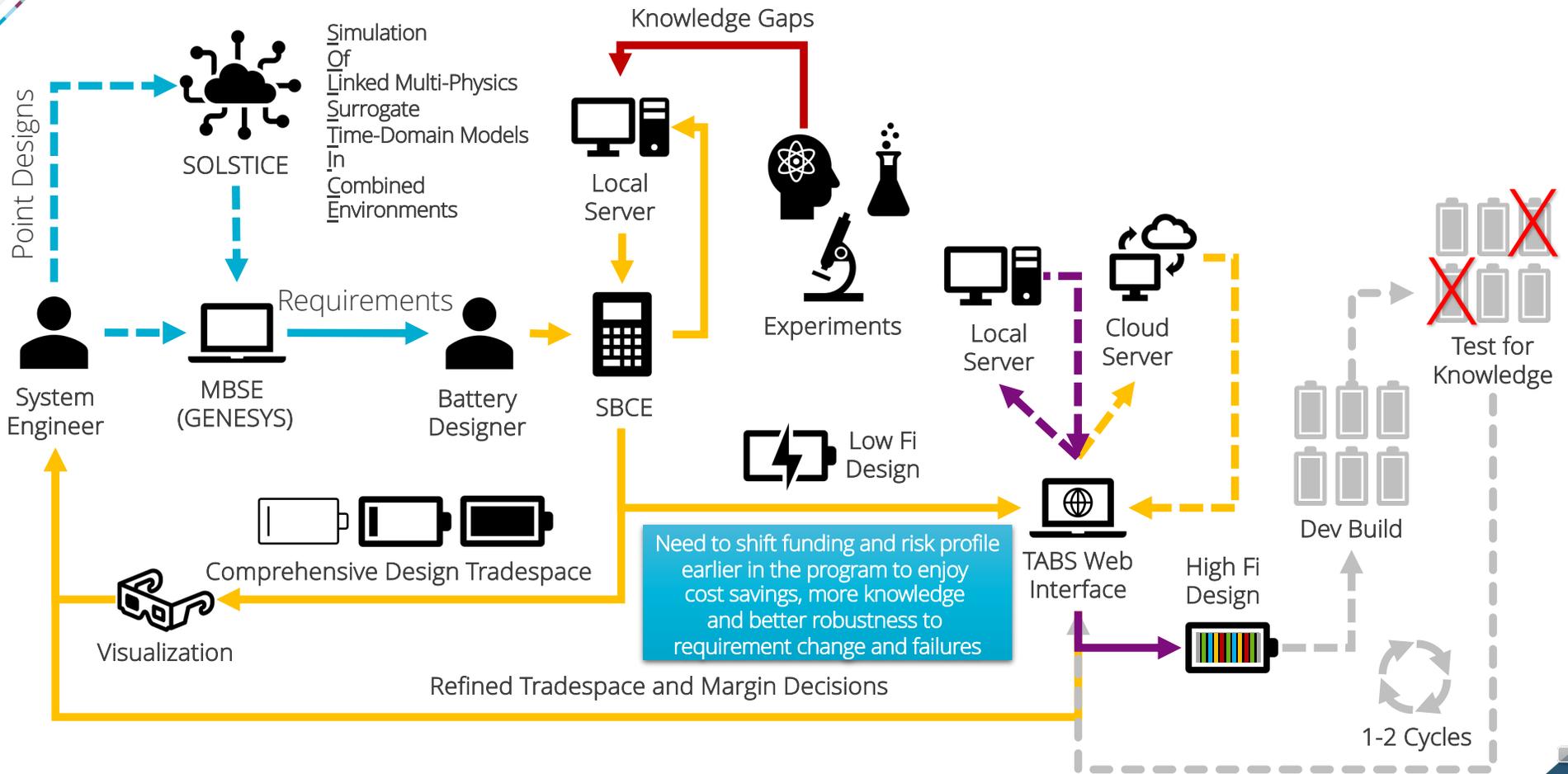
Current state of thermal battery design



Current battery design process is nowhere near optimal



Vision for accelerated digital engineering of batteries





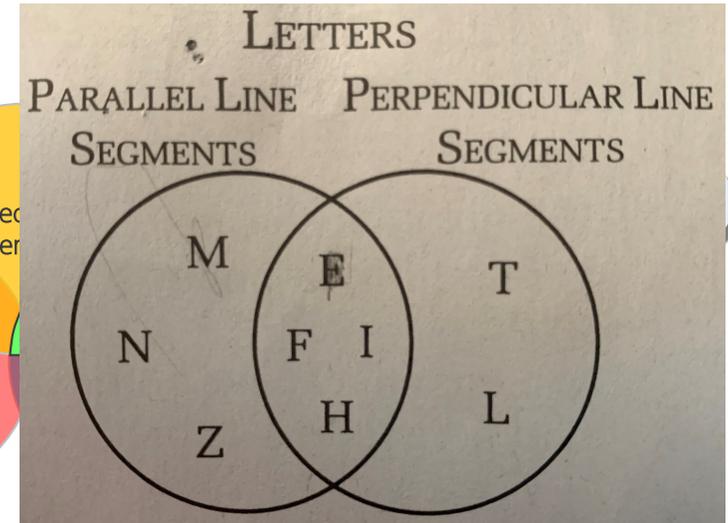
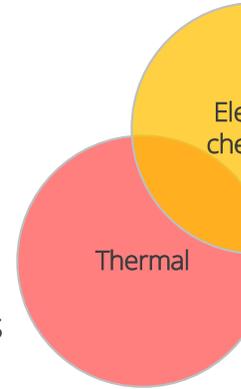
Set-Based Concurrent Engineering

What is SBCE?

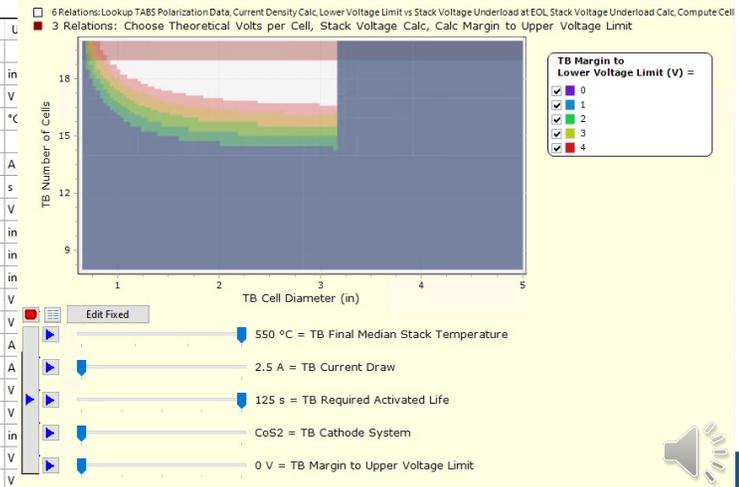
- Set-Based: Finding the set of all feasible solutions given all requirements and constraints
- Concurrent: Convergence of the set of system solutions occurs simultaneously with convergence of the set of subsystem or component solutions
- Thermal Battery team uses software called Success Assured

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



Short	Decision	U
	TB Number of Cells	L
	TB Cell Diameter	in
	TB Margin to Lower Voltage Limit	V
<None>	TB Final Median Stack Temperature	°C
	TB Cathode System	
	TB Current Draw	A
	TB Required Activated Life	s
	TB Margin to Upper Voltage Limit	V
<None>	TB Anode Thickness	in
<None>	TB Cathode Thickness	in
<None>	TB Separator Thickness	in
	TB Lower Voltage Limit	V
	TB Upper Voltage Limit	V
<None>	TB Current Density	A
<None>	TB Capacity Consumed	A
<None>	TB Cell Voltage at EOL	V
	TB Theoretical Volts per Cell	V
	TB Cell Area	in
	TB Stack Voltage Underload at EOL	V
	TB Initial Stack Voltage	V

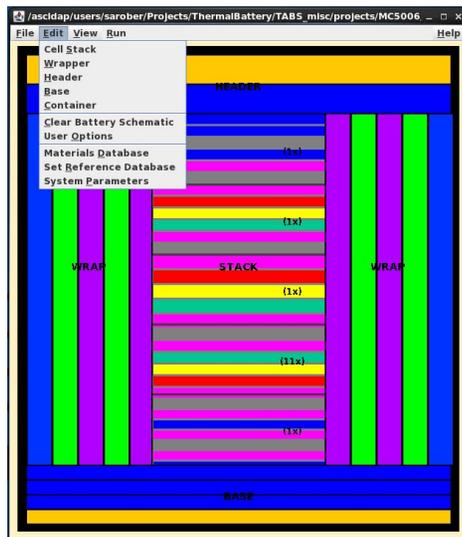




TABS: The Thermally Activated Battery Simulator

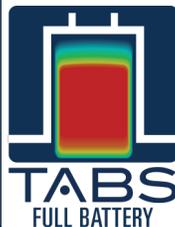
TABS design principles

- 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

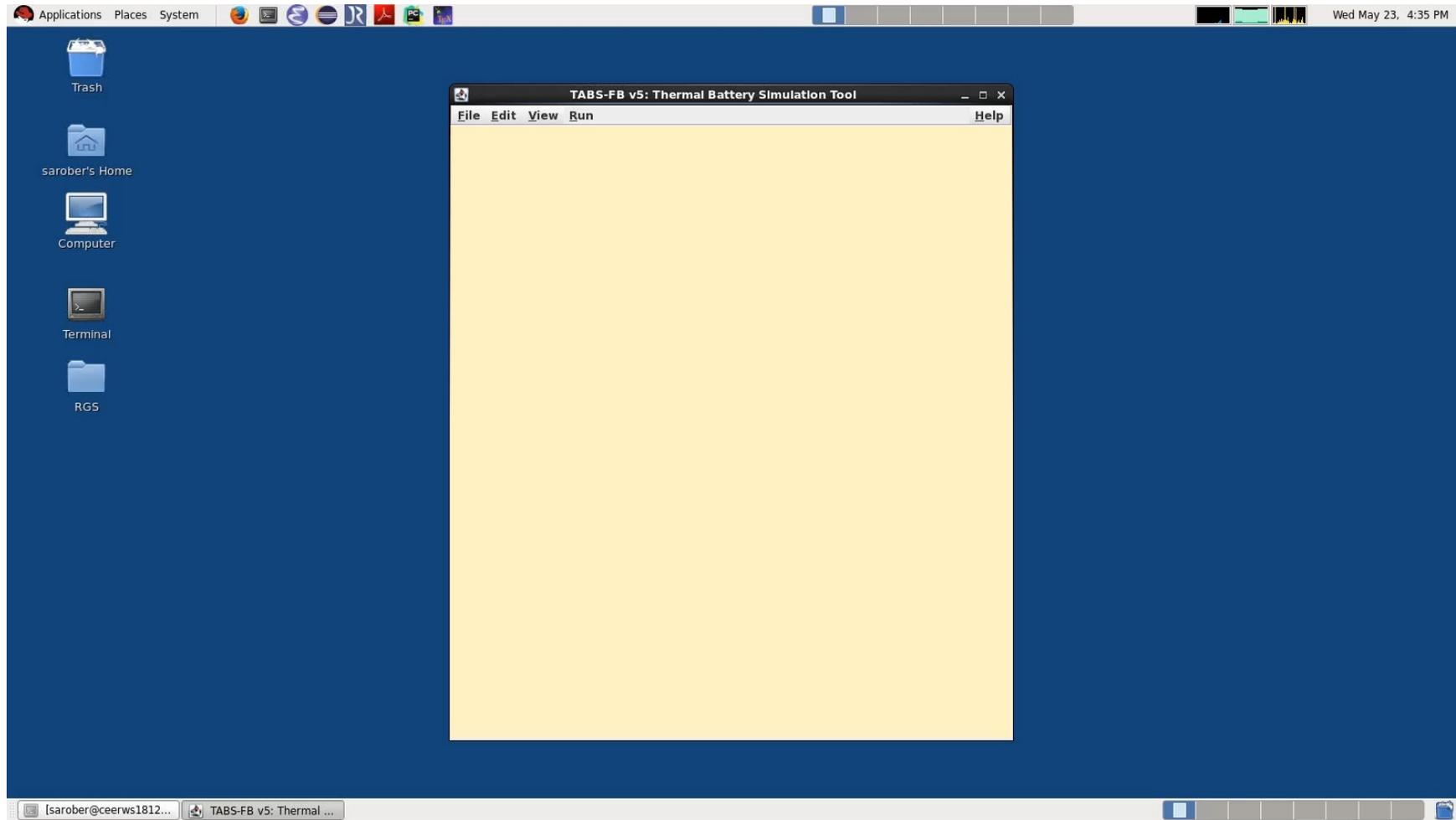
- Saved \$3.6M and 13 months of schedule on two recent life extension programs
- Cost savings recouped ASC investments to date
- Enabled first fully virtual battery design for external customer
- Yielded insight into anomalous test behavior

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

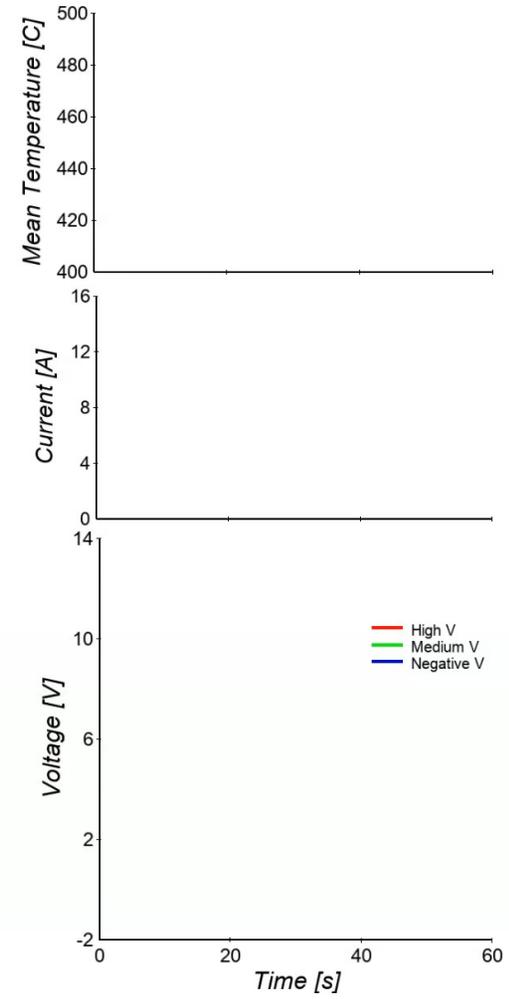
Time = 0.00 s

Current Density [A/m²]
0.0e+00 5.0e+04 1.0e+05



Temperature [C]
0 150 300 450 600

Voltage [V]
-2 2 6 10 14





Making TABs a web-based productivity tool for battery designers

The image displays a collage of screenshots from the TABs web application, illustrating its various features and user interface elements:

- Welcome to TABs:** A landing page with a "Blank Battery" button and "Battery Templates" section.
- User Materials Database:** A search interface with filters for Material Location, Material Function, and Composition.
- Battery Workflow:** A central navigation 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 Thermal Properties (Thermal Conductivity, Specific Heat, etc.) and Electrochemical Properties (Electric Conductivity, etc.).
- Summary/Preflight Check:** A panel showing battery statistics such as Size (3.3 x 5.2 Feet), Weight (12 pounds), Diameter (12 inches), Volume (100 liters), Heat Balance (12 Kcal), Current (300,000 volts), and Nominal Voltage (12).
- Full Battery:** A 3D schematic of a battery stack with various components labeled (WRAP, STACK, BASE BC) and voltage taps (Tap 3 to Tap 10).
- View Results:** A section for analyzing simulation results, featuring a "2D Plots" area with a "Tracer History" graph and "Performance Metrics" such as Average Battery Temperature (800 degrees Celsius), Maximum Voltage at each Tap (800 degrees Celsius), and Capacity Remaining (800 degrees Celsius).
- Design & Material Specifications:** A table for defining material properties and thicknesses for different groups (Insulation and Cells).

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





Making TABS a productivity tool for battery designers

The screenshot displays the 'Inside' website interface. At the top, there is a navigation bar with 'INSIDE' and links for 'Directory', 'Policy', and 'News'. A search bar is present with 'Sandia' and 'People/Orgs' filters. Below this, a secondary navigation bar shows 'Tools' and 'Topics' tabs, along with weather information for Albuquerque (49°F), a 'What's New' section, a user profile for 'Scott Roberts', and a 'Help' link.

The main content area is divided into several sections:

- Tools to get work done:** Includes buttons for 'Most Used' and 'By Category', and a list of tool categories with external links: Careers & Hiring (internal), CCHD (IT Help Desk), Common Engineering Environment (CEE), Conference Rooms, DiGS (computers, accounts), EBI Portal, EIMS FileNet, Enterprise Person, and Expense Report Plus.
- Featured Announcements:** A row of blue boxes for 'WebShipper2.0 down noon 2/25', 'Office 365 Training', 'Delve & File Sharing in O365', 'ASC S³C call for papers', 'External Thunderbird UI', and 'New! IaC via Terraform'. Below this is a link to 'View All Featured Announcements'.
- Alerts:** A prominent orange banner for 'Latest coronavirus information/FAQ and update messages'.
- Around Sandia:** A featured article titled 'Black History Month' with 11 comments, accompanied by a photo of a woman.
- Directory Quick Search:** A search box with the placeholder text 'Enter name, email, or org' and a link to 'Advanced Search'.
- My Links:** A section for personalized links with '+ Add Group' and 'Visit the My Links Tutorial' options.

A 'Feedback' button is located on the right side of the page.

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



Fully-Integrated Digital Workflow

