Sandia National Laboratories

MULTI-MODAL AI AGENTS FOR ADVANCED DATA ANALYTICS

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PROJECT PROFILE
Topic: Analytics & Tools| Vertical: Analytics
Strategic Pathway: Optimize
Project start and finish: FY26-FY27

PROBLEM

1. Challenges

- Battery data analytics demands simultaneous reasoning over **heterogeneous documents (***PDF, DOCX, TXT, CSV, XLSX, Parquet, etc.*) AND **computational tasks**, no single open-source tool handles both.
- **Degradation models** fail under **chemistry/domain shifts**, and existing platforms lack **intelligent routing** between retrieval and computation.

2. Motivation

- Explosive growth of AI data centers and grid-scale storage requires **automated, chemistry-agnostic battery analytics.**
- DOE/OE's QuESt platform is the ideal open-source vehicle to deliver **AI capabilities** at scale.

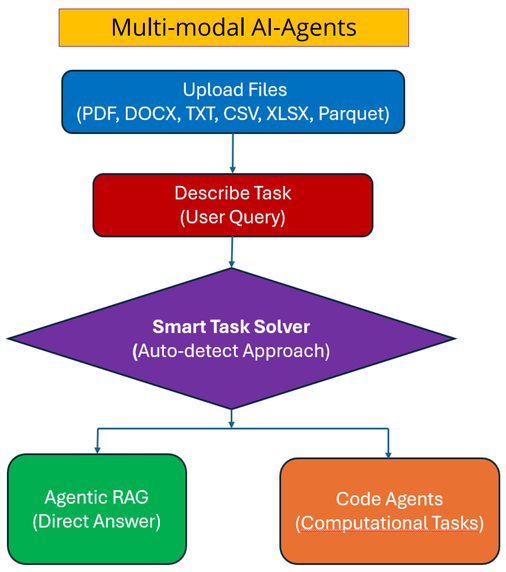
3. Current practice

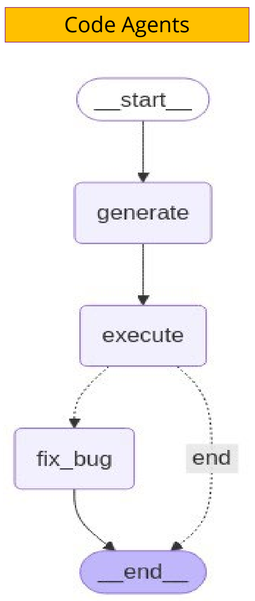
- Manual workflows and standard forecasters, e.g., Temporal Fusion Transformer (TFT) lack **uncertainty quantification under distribution and domain shifts.**
- No platform **unifies agentic RAG, code agents, probabilistic degradation modeling, and adaptive fine-tuning** in one system.

APPROACH

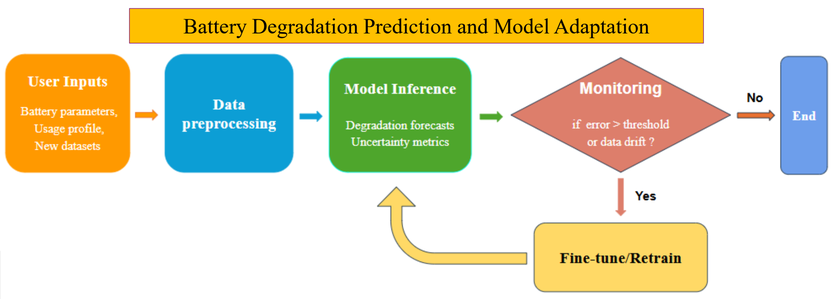
Smart Task Solver: Classifies user requests and routes them to one of two agentic pathways.

- **Agentic RAG (Retrieval-Augmented Generation):** Multi-step **document reasoning** and Question-answering (**Q&A**) across *PDF, DOCX, TXT, CSV, XLSX, and Parquet* formats.
- **AI-powered Code Agents**: Automated **code generation** from natural language, iterative **self-healing error** loop, autonomous **plot generation**, and formal **analysis report** creation.





- **Datasets**: www.batteryarchive.org
  Sandia National Labs (SNL), Underwriters Laboratories-Purdue University (UL-PUR)
- **Proposed Model:** a hybrid model of Quantile TFT (**QTFT**) with Reversible Instance Normalization (**RevIN**) technique for **probabilistic predictions** of capacity fades under **substantial distribution and domain shifts.**
- **AI-Agent frameworks**: LangChain, LangChain-OpenAI, deepagents and Streamlit.
- **Large Language Model:** GPT-4o via OpenAI API.

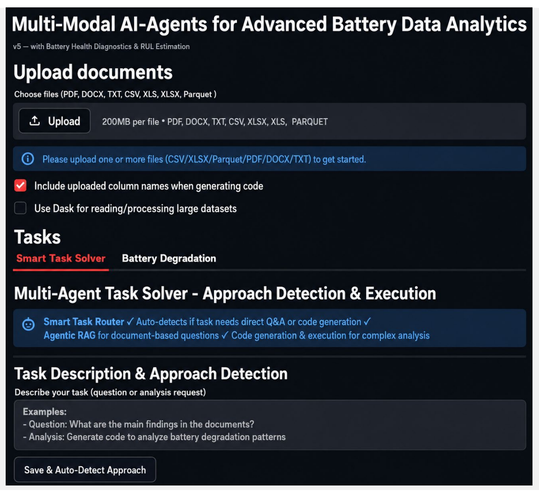


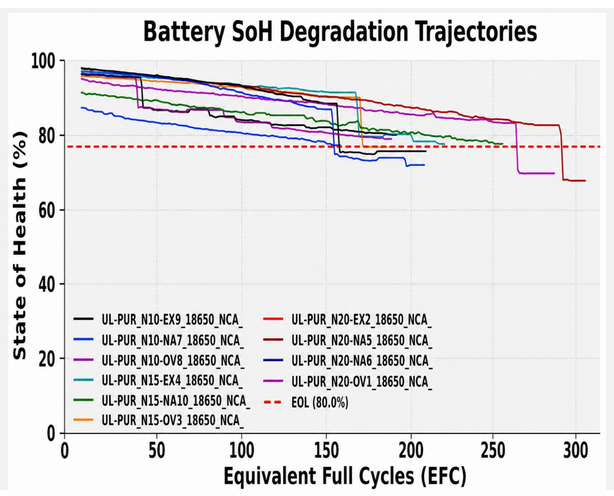
RESULTS

Case 1: AI-powered Q&A, Code and Report Generation

Key components:

- **Smart Task Solver** correctly classifies and routes diverse user requests (**document Q&A vs. computation tasks**).
- **Agentic RAG** handles multi-step reasoning across *PDF, DOCX, TXT, CSV, XLSX, and Parquet*, returning synthesized, grounded answers.
- **Code Agents** autonomously **generate, execute, debug** (self-healing loop), and produce formatted **analysis reports** and plots from natural-language queries.





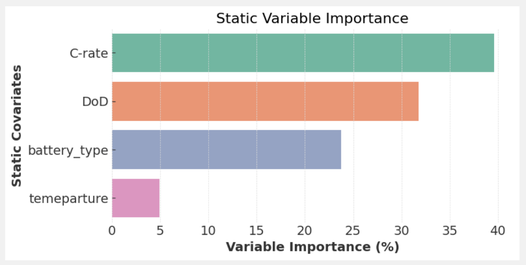
Case 2: Battery Degradation Prediction and Model Adaptation

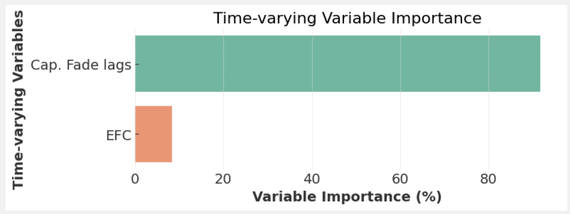
Key components:

- Hybrid QTFT-RevIN outperforms standard TFT in **probabilistic capacity-fade estimation** under **distribution/domain shifts**; demonstrated on SNL and UL-PUR datasets.
- Uncertainty quantification via quantile regression provides calibrated **prediction intervals** for battery state-of-health across **multiple chemistries**.

Table: Performance comparision of the proposed model (QTFT-RevIN) vs standard TFT model.

Model	Dataset	Retrain	MAE	MAPE	RMSE	R^2
QTFT-RevIN	SNL	No	0.04	0.04%	0.06	99.83%
TFT		No	2.63	3.04%	2.77	-11.63%
QTFT-RevIN	UL-PUR	No	0.68	0.82%	1.43	86.92%
		Yes	0.39	0.49%	1.05	90.13%
TFT	UL-PUR	No	5.55	6.23%	5.89	-127.37%
		Yes	2.93	3.40%	3.20	8.24%





CONCLUSIONS & IMPACT

- Integrated **multi-modal AI-agent capabilities** (agentic RAG + code agents + probabilistic forecasting) into one platform.
- Enables non-expert users to perform **complex battery data analytics** through natural-language interaction, lowering barriers to advanced energy storage analysis.
- The hybrid QTFT-RevIN approach advances **probabilistic battery degradation estimation** with robust uncertainty quantification under **real-world distribution shifts**.
- **Impact:** Accelerates battery research workflows, supports **data-driven decision-making** for grid-scale storage, and provides a reusable **open-source AI foundation** for DOE/OE programs.

FUTURE DIRECTIONS

- Add a **decision layer** integrating pretrained **state-of-charge (SoC), state-of-health (SoH), remaining useful life (RUL), and thermal models.**
- Incorporate **large load data-center simulations** to capture **AI data-center** energy demands.
- Implement **reinforcement learning-based dispatch policies** for optimized, explainable battery management at AI data centers and grid-scale storage.
- Extend **chemistry coverage** and enable **continual fine-tuning** as new battery datasets become available.

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