DOE Facilities: The role of advanced mathematics in meeting future needs and goals

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DOE scientific facilities will undergo radical change over the next 10-30 years. Unprecedented experimental capabilities will allow DOE scientists to greatly accelerate our ability to make scientific advances, including (1) to test, and analyze new materials to meet energy needs (solar, batteries, . . .); (2) to understand biological processes (photosynthesis, cell mechanics, proteins,. . .) for energy and health; and (3) to design and manufacture new technologies (active materials,. . .).

As examples, facilities of the future will take advantage of

- Faster acquisition and throughput, higher spatial and temporal resolution;
- Real-time analysis, robotic control of efficient, optimal experiments;
- Multi-modal multi-scale experiments across facilities and resources;
- Integrated coupling of experiment, simulation, and data analysis for rapid feedback to accelerate scientific understanding; and
- Ubiquitous computing, from local resources to seamless execution across fastest HPC resources, with shared and federated data and login

New algorithms, coupling advanced new mathematics, artificial intelligence, and data analysis, will be instrumental in providing

- Autonomous, self-driving experiments, including (a) calibrating and tuning equipment and (b) choosing and steering new experiments.
- Data analysis and computer vision across modalities, including (a) feature extraction and comparison; (b) tackling limited and expensive data; (c) classifying, archiving, and linking past, present, and future
- AI/machine learning/mathematics with embedded physics in order to (a) reconstruct and "invert" complex models; (b) iterate between observations and models; and (c) bridge gaps in multiscale modeling
- Coupled experiment and simulation to (a) extract surrogate models; (b) provide mutual feedback to refine models and interpret data

The Center for Advanced Mathematics for Energy Research Applications (CAMERA), which is jointly supported by ASCR and BES within the Office of Science, has actively been focussed on building the new mathematics, algorithms, and software required to advance these goals, including the development of the "SMART" (Surrogate Model Autonomous expeRimenT) algorithms, relying on Gaussian processes and optimization for autonomous self-driving experiment; "Mixed-Scale Dense" convolutional neural networks for image recognition and classification from limited data; "Multi-Tiered Iterative Phasing" (M-TIP) for a wide range of imaging inversion and reconstruction across a range of multi-modal experiments; and reduced order models to couple experiment and simulations.

The large amounts of data coming from these new capabilities will require, in part, significant progress on mathematical, statistical, and computer science research to quickly analyze data, perform analysis to quickly figure out where experiments are headed, and accelerate our understanding.

The range of computing, from edge computing, computing embedded next to detectors, fast connections to high-performance architectures, and seamless multi-facility computing are all key aspects of these future laboratories. Building these capabilities in tandem with advanced algorithms will ensure that state-of-the-art computing takes advantage of the coming mathematical advances in our scientific modeling and understanding.