DISCLAIMER

Basic research needs for

INVERSE METHODS FOR COMPLEX SYSTEMS UNDER UNCERTAINTY

ASCR WORKSHOP *JUNE 10TH – 12TH 2025*

U.S. DEPARTMENT OF ENERGY | Office of Science

THE IMPACT OF DEVELOPING THE MATHEMATICAL FOUNDATIONS FOR SOLVING INVERSE PROBLEMS

Inverse problems, which aim to infer unknown properties of a system using experimental and observational data, are central to many of the U.S. Department of Energy's (DOE) most critical scientific and engineering challenges. Accurate and efficient solutions to inverse problems are vital for tasks such as analyzing data from large-scale experimental facilities, optimizing fusion reactor performance, probing nuclear structure, accelerating materials discovery, identifying high-energy particle signatures, enhancing geophysical imaging, advancing tsunami early warning systems, and enabling autonomous systems and digital twins. See Figures 1-6 for examples of inverse problems in mission-critical DOE science drivers

These problems are increasingly complex, often involving nonlinear, high-dimensional, and interconnected systems and models that span multiple physics and scales, while relying on data with varying quantity, quality, and information content. Adding to these difficulties is the uncertainty found in complex systems of interest to DOE, where errors in inputs, noise in data, and discrepancies between models and reality constrain the accuracy and precision of solutions. The convergence of recent scientific computing trends—for example, scientific machine learning, artificial intelligence, and exascale computing—creates unprecedented opportunities to tackle these challenges.

The cross-cutting nature of inverse problems, combined with the rapidly evolving data and algorithmic demands of these problems, strongly motivates the formulation of a prioritized foundational research agenda to maximize their capabilities and impact. In response to this need, DOE's Advanced Scientific Computing Research program in the Office of Science convened the Workshop on Basic Research Needs for Inverse Problems for Complex Systems under Uncertainty in June 2025. The workshop brought together experts to identify grand challenges and major opportunities in the field. As a result, four priority research directions (PRDs) were identified to guide future efforts. These PRDs are summarized in this brochure, and more details can be found in the full workshop report, available at https://doi.org/10.2172/2583339.

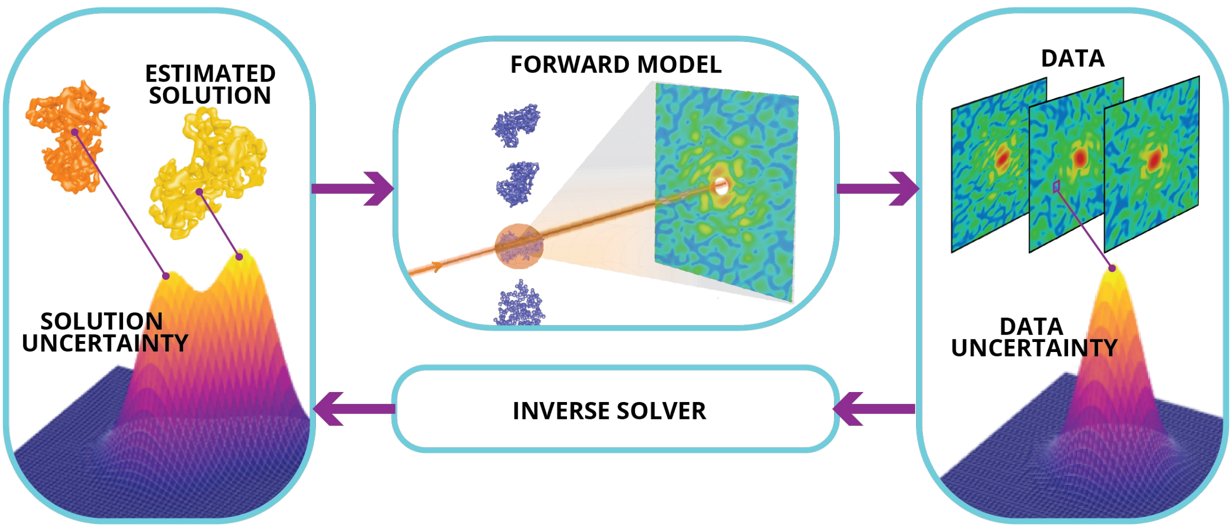

Figure 1 | Conceptual illustration of a prototypical inverse problem. Starting from an initial solution estimate, the inverse solver infers unobserved quantities of a system—the solution—from observed data by ensuring that the forward model predictions align with the data, prior knowledge, and constraints. The problem's ill-posedness, along with uncertainties in prior knowledge, models, and data, can result in multiple plausible solutions.

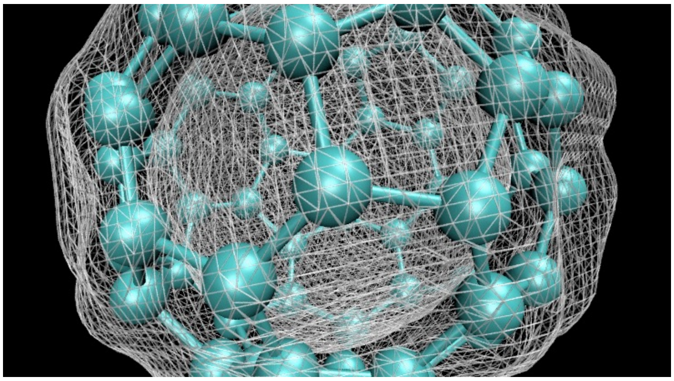

Figure 2: Reconstructing Nuclear Structure

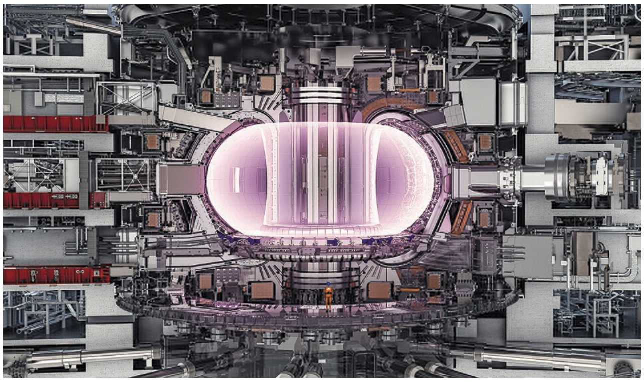

Figure 3: Inferring Plasma States of Fusion Energy Systems

PRIORITY RESEARCH DIRECTIONS

1. Discovering, exploiting, and preserving structure

Key Question: How can we exploit mathematical and physical structures in models and data to overcome ill-posedness, leverage prior knowledge, and significantly enhance computational efficiency while preserving essential properties?

Unlocking the next generation of DOE scientific discoveries will require innovative approaches for solving inverse problems that address escalating computational demands, overcome greater degrees of ill-posedness, and efficiently utilize high-performance computing and data resources. To meet this need, there are substantial opportunities to exploit new forms of mathematical, physical, and data structures inherent in emerging complex systems to reduce problem size and complexity, introduce informative priors and constraints, improve robustness and tractability, and accelerate computational performance. Achieving this will require fundamentally new methods for solving inverse problems that better leverage known structures, discover new exploitable structures, preserve essential mathematical and physical properties, and map computational and communication patterns to these structures to optimize performance on available computing and data infrastructure.

2. Identifying and overcoming model limitations

Key Question: How can we detect, quantify, and reduce model inadequacy while ensuring robust inference in the presence of imperfect likelihoods, limited simulator fidelity, and inadequate priors?

Forward models used in inverse problems are often constrained by simplified assumptions, structural discrepancies, incomplete representations of physical processes, imperfect likelihoods, limited simulator fidelity, or inadequate priors. These limitations, also known as misspecifications, compromise the reliability, efficiency, and interpretability of solutions while introducing significant uncertainty into the inference process. Addressing these challenges requires the development of mathematical frameworks to diagnose, quantify, and mitigate model inadequacy during inference. An important component of this effort will be the design of methods that provide robust uncertainty estimates consistent with the data, account for both known and unknown limitations—such as those represented by a range of possible distributions—and enhance the accuracy of inverse solutions across varying problem scales.

3. Integrating disparate multimodal and/or dynamic data

Key Question: How can we efficiently integrate multimodal and/or dynamic data across disparate scales, fidelities, and domains to maximize information gain and enable accurate, uncertainty-aware inference and assimilation?

Recent advances in data acquisition technologies have enabled measurements of complex phenomena and structures across vastly different sources, physics, domains, and scales. However, current inversion algorithms often struggle to integrate such disparate multimodal or dynamic data, which can be heterogeneous, inconsistent, and vary in fidelity, volume, and sparsity, while also contending with the use of multiple models that have conflicting representations of physics and data, or the storage and processing of data across different facilities.

Effectively utilizing disparate data, models, and facilities to solve inverse problems at DOE-relevant scales will require algorithms that capture common features in the data, filter noise, fuse multiple fidelities and scales, bridge distinct representations, and quantify correlated uncertainties. Methods are also needed to dynamically assimilate data, update rapidly evolving posterior distributions, and address abrupt changes in nonlinear, multiscale, multiphysics, or chaotic systems.

4. Solving goal-oriented inverse problems for downstream tasks

Key Question: How can goal-oriented inverse problems (GIPs) be formulated and solved to optimize the allocation of data and computational resources and tune accuracy and uncertainty estimates to downstream tasks?

Inverse problems have traditionally focused on inferring model parameters from data, but they are increasingly being integrated into downstream tasks such as control, design, certification, and decision support. This shift creates a pressing need for goal-oriented inverse problems (GIPs), which reformulate inverse problems to directly align with the objectives of downstream tasks, enabling improved predictions, reduced uncertainty, and enhanced decision-making for complex systems on actionable timescales. Realizing the potential of GIPs will require the codesign of scalable algorithms for inverse problems and downstream tasks, including methods to quantify uncertainty in task outcomes, exploit parameter-to-task relationships, autonomously steer experimental data collection, efficiently allocate computational resources, adapt model structure or fidelities, support "what-if" decision-making, and implement risk-aware approaches tailored to stakeholder needs.

SUMMARY

The four priority research directions outlined in this brochure represent a cohesive vision for advancing the science of inverse problems for complex systems under uncertainty. Together, they address the critical challenges of: discovering, exploiting, and preserving physical and problem structure; overcoming model limitations; integrating disparate, multimodal, and/or dynamic data; and tailoring the solution of inverse problems to downstream tasks. While each PRD focuses on a distinct aspect of inverse-problem research, their interconnected nature highlights the importance of a holistic approach that leverages progress across all areas to achieve transformative solutions. This agenda calls for research across mathematics, statistics, and computer science disciplines, which are guided and complemented by rapid advances in artificial intelligence, high-performance computing, and experimental facilities, to unlock new capabilities, maximize scientific impact, and meet the growing demands of inverse problems that arise across applications that are critical to DOE's mission.

FIGURE CREDITS

Figure 1 | Reconstruction of a 3D protein structure from a large number of 2D single-particle diffraction images measured in an X-ray free-electron laser experiment. Image courtesy of Jeffrey Donatelli, Lawrence Berkeley National Laboratory.

Figure 2 | Calibration of nuclear energy density functionals is an inverse problem where a controlled set of design parameters is adjusted to match experimental data. Image credit: Isaac Tamblyn, University of Ottawa, shared under the Creative Commons license: https://en.wikipedia.org/wiki/en:Creative_Commons.

Figure 3 | Precise control of fusion systems requires inferring plasma states from observational data. Image credit: Oak Ridge National Laboratory, shared under the Creative Commons license: https://en.wikipedia.org/wiki/en:Creative_Commons.

Figure 4 | Inference of Higgs boson properties from observed high-energy particle-collision events. Image credit: Conseil Européen pour la Recherche Nucléaire.

Figure 5 | Model domain used to infer the properties of tsunamis in the Cascadia subduction zone used for implementing early warning systems. Image courtesy of Omar Ghattas, University of Texas at Austin.

Figure 6 | High throughput femtosecond laser fabrication and characterization used to produce desired target optical properties. Image courtesy of Juliane Mueller, National Renewable Energy Laboratory.

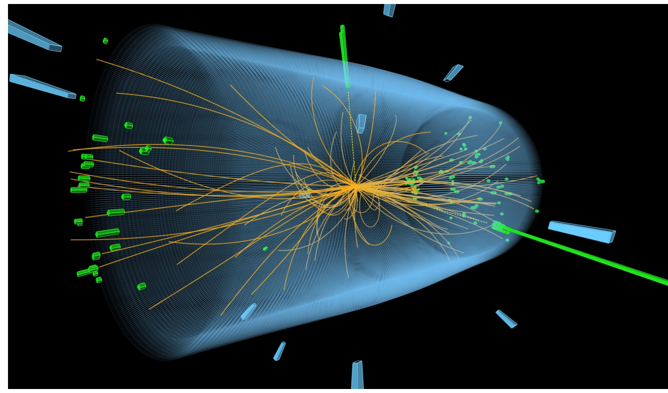

Figure 4: Inferring New Fundamental Particle Properties

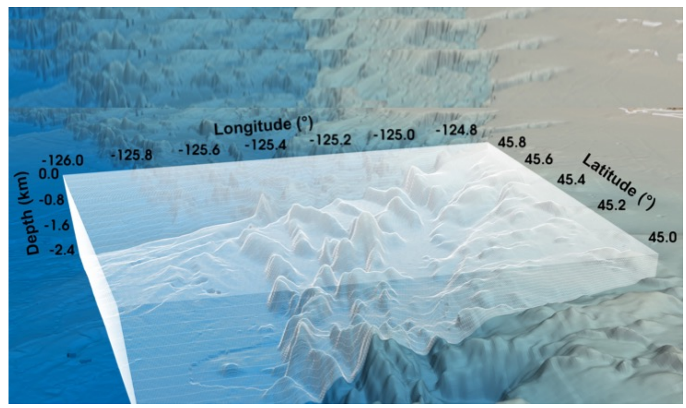

Figure 5: Tsunami Source Characterization

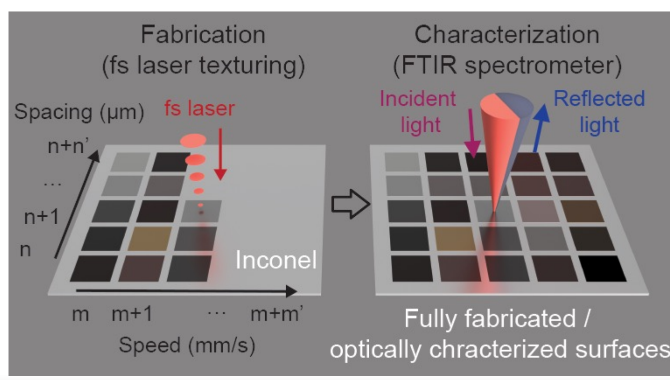

Figure 6: Inverse Design of Materials

U.S. DEPARTMENT OF ENERGY | Office of Science