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Data- and Mechanism-Driven Hybrid Computing: A New Paradigm for Scientific and Engineering Computation

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Abstract. Data- and mechanism-driven hybrid computing refers to the integration of traditional mechanism-based computing with data-driven methods. In this article, we present three typical patterns of this emerging paradigm: (1) mechanism-driven model optimization via data-driven refinement, (2) data-driven model construction with physical constraints, and (3) alternating optimization of mechanism-driven and data-driven models. We present several concrete examples to illustrate how hybrid computing improves accuracy, efficiency, and robustness across a variety of computational tasks.

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Key words: Data-driven methods, mechanism-driven models, hybrid computing.

1 Introduction

Scientific and engineering computations primarily serve four key purposes: perception, design, prediction and comprehension. Over the past few decades, researchers have developed a wide range of algorithms to address various problems aligned with these goals, applying them to real-world domains such as oil exploration, structural design, weather forecasting and materials modeling. Traditionally, these computations rely on mathematical models such as partial differential equations (PDEs) to capture physical mechanisms,

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and utilize numerical solvers and optimization techniques for computation [16,65]. More recently, the rise of machine learning has introduced a data-driven paradigm, offering new approaches to modeling and computation that have significantly advanced the field of scientific computing [22]. Before delving deeper, we briefly outline these four objectives as follows:

1. Perception. Perception involves extracting information about the environment or a given situation from measurement data. For instance, in oil exploration, inverse problems are solved to infer subsurface properties of the Earth – such as the spatial distribution of reservoirs-based on indirect measurements like seismic waves or electromagnetic fields [81]. Another representative example is situation awareness (SA) [23], where the goal is to construct a comprehensive understanding of the current and near-future state of an environment and its components. This understanding can then support informed decision-making and strategic planning in various domains, such as military operations or traffic control systems.

2. Design. Design tasks utilize computer simulations to assist in creating, modifying, analyzing, or optimizing engineering systems. These tasks are widely applied in the field of computer-aided design (CAD) [35]. For instance, in bridge engineering, finite element analysis can predict structural behavior under different loads and environmental conditions. Such predictive capabilities enable engineers to fine-tune design parameters to ensure compliance with safety and performance standards.

3. Prediction. Prediction focuses on forecasting the future evolution and state of dynamic systems. A prominent example is numerical weather prediction (NWP) [13], which simulates atmospheric dynamics using fluid mechanics equations to generate reliable weather forecasts several days or even weeks in advance.

4. Comprehension. Comprehension leverages numerical computation as a powerful tool for developing physical models that align with experimental observations. For example, in molecular simulations, potential energy surfaces of materials are constructed by fitting both ab initio calculations and experimental data [77]. These surfaces enable a deeper understanding of material behavior at the atomic level. Building upon this, molecular dynamics simulations can further uncover fundamental mechanisms underlying physical phenomena such as phase transitions.

Across these computational tasks, methods are commonly evaluated based on three key attributes:

1. Accuracy. It refers to how closely the computational results match the true values.

2. Efficiency. It measures the computational resources such as time and memory.

3. Robustness. It indicates the method's ability to perform reliably under varying conditions, such as changing parameters, model uncertainties or noisy data.