QUANTUM INNOVATION 2023

CP-04-02

Quantum CAE: automation in science with quantum computing and machine learning

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Abstract

Scientific discoveries progress through experimentation, data processing, and the formation of new hypotheses. Recently, advancements in computer capabilities and algorithmic enhancements have enabled the partial automation of this process, a trend particularly noticeable in Computer-Aided Engineering (CAE) within the industrial sector. In CAE, simulations are utilized to extract product characteristics (observable values) from blueprints (hypotheses), subsequently refining the blueprints based on these characteristics. From a machine learning perspective, this equates to input and output data. As more data becomes available, it becomes feasible to construct a surrogate model that represents this relationship. Solving the inverse problem of this model provides the desired blueprints (hypotheses). Optimization techniques play a crucial role in solving the inverse problem, indicating that product design with CAE is a cyclical process involving simulations, machine learning, and optimization. Studies have demonstrated that these computational tasks are well-aligned with the strengths of quantum computers, and it is anticipated that they will substantially reduce the lead time for producing product blueprints. Quantum CAE, defined as performing these tasks on a quantum computer, not only accelerates the process but also aids in automating science, reflecting the cycle of scientific discovery and promoting a more efficient and innovative approach.