Mixed-Integer PDE-Constrained Optimization

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Exascale platforms offer unprecedented opportunities for a paradigm shift from traditional forward simulations to design and optimization of complex structures, thereby transforming computational science into a truly predictive science. A growing class of optimal design and operational problems involve the combination of complex PDE simulations, uncertainty, and a mixture of discrete (or integer) and continuous design parameters, giving rise to what we term *mixed-integer PDE-constrained optimization problems* (MIPDECOs). This new class of problems requires the integration of three mature areas of applied mathematics, namely PDE-constrained optimization (PDECO), mixed-integer optimization, and uncertainty quantification. An integrative approach is key to making solutions of these classes of problems accessible at the exascale, where algorithms must exploit and address unprecedented levels of concurrency, architectural hierarchy, and faults.

Optimal Design Applications within DOE. There exists a wealth of optimal design applications that can be modeled as MIPDECOs within DOE.

- The remediation of contaminated sites, extraction of oil and natural gas, and carbon sequestration result in complex optimization problems, where operational cost is minimized subject to constraints on subsurface flows. Uncertainties arise in modeling the unknown state of the subsurface, and integer design parameters model the location and operation of wells.
- The strategic goal to transform the nation's energy systems to 80% clean energy by 2035 creates many opportunities for optimal design. The design of nano-materials for ultra-efficient solar cells involves the solution of Maxwell's equation; integer parameters model design choices; and uncertainties arise due to manufacturing variabilities. The optimal placement and control of wind farms involves fluid dynamics simulations based on Navier-Stokes equations; integer parameters model turbine selection/activation and placement; and uncertainties are environmental or due to material wear and tear.
- The operational planning for nuclear reactors combines complex simulations that combine neutron transport and fluid flow models with integer decisions on the arrangement of fuel rods. Uncertainties are associated with imperfect knowledge of the fuel.

Each of these problems is itself a grand-challenge problem with the potential to transform an application area. By abstracting these applications mathematically as MIPDECOs, we can develop a new set of algorithmic approaches with the potential to transform applications across DOE.

A New and Challenging Class of Mathematical Problems. Formally, we can define MIPDECOs as

$$\underset{y(\gamma),u,z}{\text{minimize}}\ F(y(\gamma),u,z) \quad \text{subject to } g(y,u,z;\gamma)=0,\ \forall\gamma\in\Gamma, \quad \text{and } y\in\mathcal{Y},\ u\in\mathcal{U},\ z\in\mathbb{Z}^p\cap S,$$

where $y(\gamma)$ are the state variables that depend on the random variables $\gamma \in \Gamma$, u are the continuous design variables, z are the integer design variables, and g describes the PDE. This new class of problems builds on PDECO, uncertainty quantification, and mixed-integer optimization, and results in a broad set of mathematical and computational challenges.

Hierarchical Mixed-Integer Techniques for MIPDECO. Traditionally, mixed-integer problems are solved by using a tree search. However, three fundamental mathematical challenges for

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MIPDECO imply that this approach is unlikely to be successful. First, the search tree of even a simple MIPDECO is huge, involving potentially millions of binary variables. Second, every node of the tree corresponds to a PDECO, whose computational cost is equivalent to the cost of several forward PDE solves. Third, the performance of the system is influenced by uncertainty that must be accounted for in the final design.

To tackle these challenges, we must develop an integrated algorithmic strategy. We must more efficiently integrate PDECO and PDE solves in the tree search and develop bounds for these inexact solves in order to ensure efficient pruning during the tree search. We must explore tree-search techniques based on surrogate models that can be tuned with just a handful of forward solves and the corresponding derivatives/adjoints. These surrogates provide a coarse approximation of the physics useful for searching the tree that can be efficiently propagated up a machine's hierarchy. We must develop hierarchical methods that extend recent multilevel techniques for combinatorial optimization and integrate these with continuous multilevel optimization ideas in order to align algorithmic hierarchies with machine hierarchies. Finally, we must allow the optimization framework to guide the exploration of the uncertain parameters as the optimal design is approached. Only by understanding the full breadth of mathematical models that MIPDECO entails can methods fully exploit an exascale's machine heterogeneous memory and communication hierarchies.

Integrated Uncertainty Quantification. In applications, uncertainty arises from many sources. Examples are errors from bulk measurements of material properties (e.g., permittivity, permeability), manufacturing inaccuracies, and numerical/modeling errors in terms of coarse discretization, inaccurate linear or nonlinear solutions, improper boundary conditions, under-resolved material property variations, or errors from data measurements in the case of inverse problems and model calibration. A promising approach to tackle these problems is to combine PDECO with stochastic programming approaches and view uncertainty in the context of a two-phase stochastic mixed-integer optimization problem. The first phase addresses the design variables, and the second-phase variables are solutions to the stochastic PDE parameterized by the first-phase variables. An integrated approach to handling uncertainty offers unprecedented potential for stochastic dimension reduction, based on combining adjoints with goal-adaptive optimization methods.

Toward Billion-Way Concurrency. An important aspect of our integrative approach is ensuring that the robust integration of the mathematical models and algorithmic tools maps well to the massive concurrency projected at the exascale. MIPDECO offers three hierarchical levels of parallelism: the linear solver level, the PDECO level, and the mixed-integer tree-search. At the highest level we operate a tree search, where every node in the tree represents an optimization problem, which in turn requires a series of PDE solves. The tree can be searched asynchronously in parallel, and such approaches have scaled to 1,000 parallel tree-searches. The presence of uncertain parameters offers another, independent opportunity for parallelization by applying decomposition schemes that result in loosely coupled forward solves. Finally, the optimization and forward PDE solves are themselves highly parallelizable. These parallel opportunities are largely independent of one another, promising multiplicative performance gains suitable for extreme-scale architectures.

Algorithm-Level Resiliency. Resiliency and reduced mean-time-to-failure are growing concerns for exascale platforms. Where current checkpoint-restart approaches are not practical, our approach to MIPDECO must provide algorithms that are inherently resilient to hard and soft errors. Optimization frameworks such as trust-region methods offer a high-level approach to resilience that can detect applicable errors or failures at negligible computational cost. Similarly, tree-search strategies offer efficient local checkpointing techniques that can be further enhanced by exploiting the multilevel hierarchy of the algorithms.