PSAAP IV Research Topic: Design Optimization

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Executive Summary

Design optimization entails the development or usage of mathematical formulation to inform the selection of an optimal material or system design. This can be applied to a wide range of applications, and those of most interest to the Advanced Simulation and Computing (ASC) Program include physics and engineering applications that encompass both a wide range of physics and scales. Thus far, the majority of optimization efforts have focused on linear elastic, quasi-static and steady-state problems. **The computational complexity and resource requirements for nonlinear (including irreversible) and dynamical behavior remain the major hurdle in exploring and discovering creative and non-intuitive novel designs**. As an example, a single forward analysis using the finite element method for the design of highly non-linear phenomena (e.g., crash dynamics) can take a week or more on current high-performance computing (HPC) architectures. Thus, the repetitive application for hundreds of iterations of such an approach to compute gradients and optimize a design is prohibitive. The state-of-the-art to address these problems includes determining a series of equivalent static loads which are then optimized for multiple load cases. This approach neglects dynamic effects and nonlinear behavior, and hence, does not result in the truly optimal design.

This research topic addresses such challenges by focusing on the development and application of novel optimization techniques aimed at **Inverse Design** and/or **Shape/Topology Optimization**, which are described in more detail below. Given the complexity of multiple scale nonlinear design problems, it is critical that the latest state of the art computational science and computer science be brought together to enable an integration of high-fidelity coupled modeling and inverse optimization in order to discover novel and unintuitive designs to achieve unprecedented performances.

Inverse Design

Inverse design provides the opportunity to develop new material and system designs that can exhibit enhanced and/or tailored properties. Key challenges lie in the inverse design of high-dimensional (material) systems, that include multiscale mechanics, irreversible/destructive waves and/or nonlinear wave-defect interaction. As described above, design optimization for dynamics has, so far, studied linear, frequency domain problems. This greatly limits the power of inverse design for a wide-range of systems of interest to the ASC Program that include complex and multi-physics loading conditions, multiscale and large-scale systems, and dynamic conditions.

We invite proposals in the following areas:

- **Realizing process-structure-property (PSP) relationships** is still a premier challenge, particularly when considering new advanced manufacturing technology. It is known that constituent properties of the materials forming the metamaterials' small-scale structures dictate their total effective property, making this an inherently multiscale/large-scale challenge. Additive manufacturing (AM) provides an example in which design optimization can account for uncertainties associated with the AM material properties. Combining techniques such as design optimization, multiscale mechanics for PSP, and the latest uncertainty quantification (UQ) methods provides new opportunities for realizing novel metamaterials. However, such an approach requires huge computational resources. Therefore, there is a need, and outstanding challenges to overcome, to bring together the latest state-of-the-art computational and computer sciences in these areas (i.e. design optimization, PSP and UQ).
- **Design optimization with machine learning (ML)** is an approach that has promise for all computationally expensive problems. While there has been a recent surge of successful approaches that address PSP modeling and UQ with ML, there are still grand challenges in incorporating design optimization into this workflow. Specifically, design optimization has the standing challenge that our understanding of optimum designs is highly limited and there is usually not enough data of optimized designs for training. Thus, careful consideration and formulation of design optimization algorithms with ML requires major research efforts. In recent cases where design optimization methods combining ML and conventional optimization have been successful, the approach has again only been applied to linear elasticity and straightforward energy minimization.
- **Nonlinear mechanical phenomena** are unavoidable in applications requiring light-weight failure-tolerant components, energy absorption, and elastomeric materials for vibration suppression. Recent works have begun in designing novel metamaterial/metasurfaces that utilize considering optimization-based design with failure incorporated through nonlinear mechanics models such as plasticity and fracture, but much more work is needed to achieve robust and efficient formulations for solution of realistic problems. Similarly, much effort has been devoted to design of elastomeric materials undergoing large deformations and snap-through instabilities, but more work is needed to incorporate viscoelastic constitutive behavior and contact. Design optimization for dynamics has, so far, studied linear, frequency domain problems. Thus, there are currently no design rules or tools for more complex dynamical behavior in high-strain (e.g. shock) and irreversible regimes and their predictability is highly limited. Inverse design methods (possibly with ML) can be used to search for the macroscopic material behaviors that meet targeted design requirements, followed by shape/topology optimization to realize the microstructures that provide the desired material response.

Shape/Topology Optimization

Topology and Shape Optimization promise novel approaches for design, test, and production, particularly when dealing with combined physics environments, high-frequency wave propagation, and nonlinear mechanics where the simulation codes may be costly and manifest non-obvious behavior. While the National Labs have made substantial investments in large-scale modeling and simulation codes, promise of these codes as design tools remains largely unrealized for their primary missions.

Given the extremely large number of variables involved in general shape- or topology-design problems, it is essential to use gradient-based optimization methods with a tight coupling to the underlying physics codes, which must be appropriately instrumented to compute objective and constraint functions, and their gradients. Users need to be able to constrain allowable shapes and topologies in an intuitive way, with an eye towards manufacturing processes.

We invite proposals in the following areas:

- **CAD to mesh:** traditionally, geometry description, meshing, and physics simulation have been developed independently. By the time the mesh is given to the physics code, the underlying geometry and the sensitivity of the mesh to that geometry have been lost. Particularly welcome are proposals that leverage existing commercial software and avoid wholesale rewrites of meshing and simulation codes.
- **Mesh to CAD:** methods for automatic construction of CAD models from faceted surface descriptions. This can be considered not only a post-processing step for topology optimization, but also a means of identifying suitable parameterizations for evolving surfaces in shape optimization.
- **Mesh maintenance:** maintaining mesh quality is a challenge both for free-form shape optimization and for topology optimization based on level-set methods that slice up a background mesh. Solutions should be robust and tied to the underlying geometry.
- **Constraint formulations:** general shape optimization problems require constraints on surface smoothness, symmetry, and manufacturability. Stress constraints or other state constraints that are not purely geometric may also be in play. Another challenging class of constraints is that of contact constraints, i.e., constraints to prevent disjoint pieces of the structure from coming into contact as the shape is changed. These constraints must be formulated in a way that facilitates the solution of the overall optimization problem.
- **Designs involving a high density of surfaces** (e.g. gyroids) is one class of mechanical metamaterials that is both challenging for conventional topology optimization and have potential usefulness to a wide range of applications. The behavior of such material systems is most accurately modeled by thin-shell elements and the common topology or design optimization approaches do not immediately apply partly because this class of problem is inherently nonlinear, and also because existing optimization methods can only search within an extremely restricted design space.

References for state-of-the-art

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