Los Alamos NATIONAL LABORATORY

PSAAP IV Research Topic: Design Optimization

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Design Optimization

- 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 problems, and the ASC Program is particularly interested in physics and engineering applications that span a wide-range of (length and time) scales and encompasses complex physics.
  - This topic is focused on two key areas: **Inverse Design** and **Shape/Topology Optimization.**

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.

Inverse Design

- Provides the opportunity to develop new material and system designs that can exhibit enhanced and/or tailored properties.
- Application interests: complex and multi-physics loading conditions, multiscale and large-scale systems, and dynamic conditions.

- **Realizing process-structure-property (PSP) relationships**
  - Constituent properties of the materials forming the (meta)materials' small-scale structures dictate their total effective properties.
    - This an inherently multiscale/large-scale challenge.
  - Opportunities to bring together design optimization, PSP, and uncertainty quantification (UQ)
    - Typically these approaches require huge computational resources, so there is room to combine state-of-the-art techniques and also novel computer science.

Inverse Design (continued)

- **Design optimization with machine learning (ML)**
  - Recently there has been a surge of work in this area, particularly when connecting PSP and UQ.
  - Standing challenge that our understanding of optimum designs is highly limited and there is usually not enough data of optimized designs for training.
  - Recent successful application of design optimization and ML still are applied to linear elasticity and straightforward energy minimization
    - Standing challenge of addressing nonlinearities, complex systems, and dynamic behavior.

- **Nonlinear mechanical phenomena**
  - Unavoidable when considering realistic (meta)materials and systems.
    - Plasticity, damage, fracture, light-weight failure-tolerant components, energy absorption, elastomeric materials for vibration suppression, etc.
  - 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.
  - Potential for broad integration of themes:
    - 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

- Promises novel approaches for design, test, and production, particularly when dealing with combined physics environments, high-frequency wave propagation, and nonlinear mechanics where simulation codes may be costly and manifest non-obvious behavior.
- Application interests: utilizing and extending well established codes as robust design tools.

- **CAD to mesh**
  - Traditionally, geometry description, meshing, and physics simulation have been developed independently
    - Underlying geometry and related sensitivities can be lost during physics simulations.
  - It is attractive to look to possibilities with commercially available code.

- **Mesh to CAD**
  - Methods for automatic construction of CAD models from faceted surface descriptions.
    - Can be a means of identifying suitable parameterizations for evolving surfaces in shape optimization.

Shape/Topology Optimization (continued)

- **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 could also be possible.
  - An open challenge is 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.

Shape/Topology Optimization (continued)

- **Designs involving a high density of surfaces**
  - Class of mechanical metamaterials that is both challenging for conventional topology optimization and have potential usefulness to a wide range of applications.
    - Most accurately modeled with thin-shell elements
  - 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.

Summary

- Development and advancement of novel design optimization techniques has the potential for wide-reaching and high impact both within the Laboratories and broadly within the scientific community.
- Focus areas: Inverse Design and Shape/Topology Optimization
- Open challenges: addressing nonlinearities, complex systems, and dynamic behavior

Given the complexity of multiple scale nature of nonlinear mechanical metamaterial design problems outlined above, it is critical that the latest state of the art computational science and computer science 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.

Thank you!