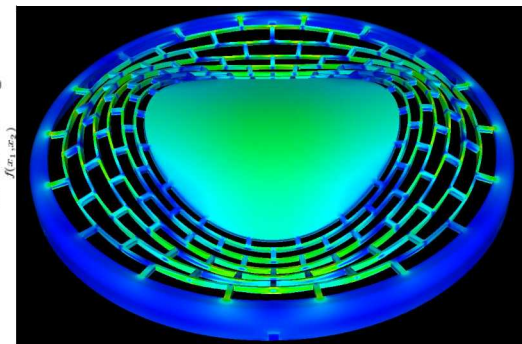
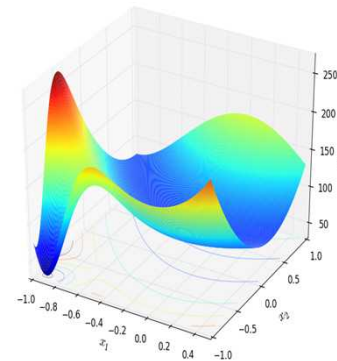


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A Second-Order Accurate Mathematical Optimization Algorithm Based on Gradient Information

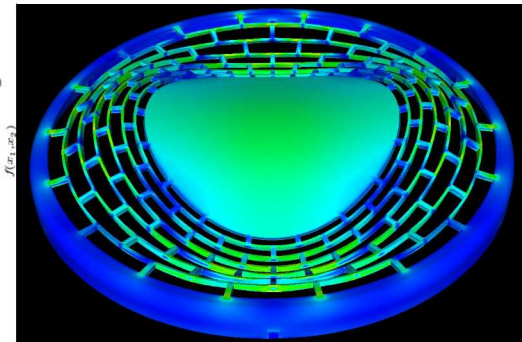
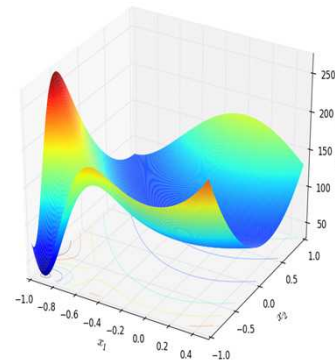
Miguel A. Aguiló

July 29, 2015

Agenda

- Motivation
- Proposed Methodology
- Optimization Algorithm
 - Pseudocode
 - Hessian Information Approximation
- Examples
- Future Research Directions
 - Conclusions

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Motivation



Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

■ Optimization Algorithmic Research

- Reduce computational expense of topology optimization problems
- Minimize tuning parameter
- Investigate effectiveness of multiple optimization algorithms in the context of topology optimization

■ Questions

- Can second-order information reduce computational expense of topology optimization problems?
- Can we minimize the computational cost associated with computing second-order information?

Proposed Methodology

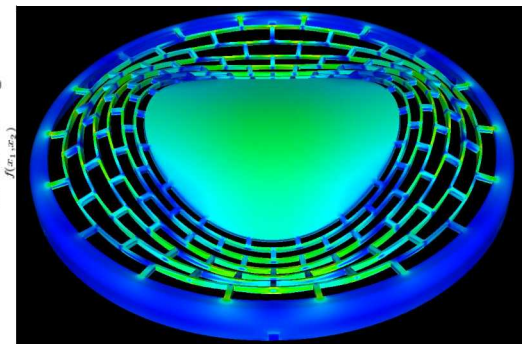
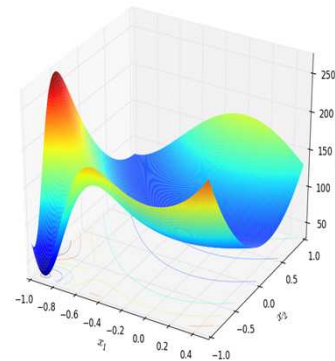
- **Objective:**

- Develop a general optimization algorithm that enables the computation of *second-order* (i.e. *Hessian*) information from the available *first-order* (i.e. *gradient*) information

- **Requirements:**

- Second-order derivative operators are not required
- Computational cost does not increase with the number of design variables
- Computational cost is the same as solving the topology optimization problem with just gradient information

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Optimization Algorithm



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Algorithm Pseudocode

Outer Loop

```
Set initial  $x_{i=0}$   
Compute  $J(x_{i=0})$   
while(not converge)  
{  
    Solve Sub-problem  
    Check convergence  
     $i=i+1$   
}
```

Legend

x = Control
 J = Objective function
 G = Gradient
 H = Hessian
 d = Trial step

Line Search Sub-problem

```
{  
    Compute  $G(x_i)$   
    Apply filter  $F(G_i)$   
    Solve  $H(x_i)d_i = -G(x_i)$   
    Line search scaling  $s_i$   
     $x_{i+1} = x_i + s_i d_i$   
}
```

Trust Region Sub-problem

```
while(TR criteria met)  
{  
    Compute  $G(x_i)$   
    Apply filter  $F(G_i)$   
    Solve  $H(x_i)\tilde{d}_i = -G(x_i)$ ,  $\tilde{d}_i = s_i d_i$   
    Check TR sub-problem convergence  
        -  $x_{i+1} = x_i + \tilde{d}_i$   
}
```

Hessian Approximation: Finite Differences (FDiff)

Finite Difference

Given $h > 0$, the d^{th} order derivative of an univariate function $f(x)$ can be approximated by finite differences as follows:

Forward
$$\frac{h^d}{d!} F^d(x) + O(h^{d+p}) = \sum_{i=i_{\min}}^{i_{\max}} C_i F(x + ih)$$

Backward
$$(-1)^d \frac{h^d}{d!} F^d(x) + O(h^{d+p}) = (-1)^d \sum_{i=i_{\min}}^{i_{\max}} C_i F(x + ih)$$

Centered = *Forward* - *Backward*

where $p > 0$ denotes the order of accuracy, i_{\min} and i_{\max} denote some choice of extreme indices, and coefficients C_i

Cont: Finite Difference

Example

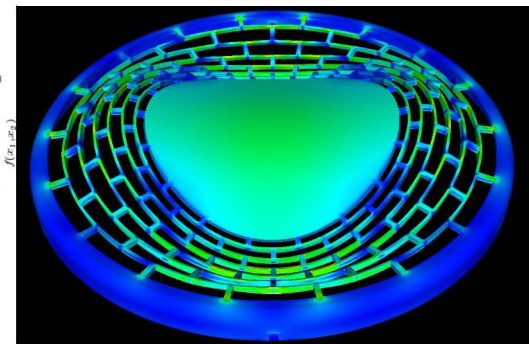
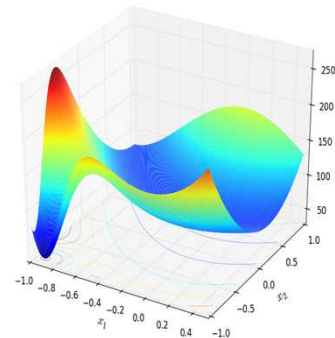
Given gradient operator $G(x_i)$, approximate the application of the trial step to the Hessian operator, i.e. $H_i(x_i)d_i$ through finite differences as follow

Backward
$$G'(x_i) = \frac{3G(x_i) - 4G(x_i - hd_i) + G(x_i - 2hd_i)}{2h} + O(h^2)$$

Key Features

- Full Hessian operator is not assemble
 - Interested in the application of the trial step to the Hessian operator
- Each evaluation is independent and thus parallelizable
 - Task parallelism can be effectively employ to expedite computation

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Examples



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Case Study: Compliance Minimization

Optimality Criteria (OC) Formulation

$$\begin{aligned} & \min \quad \frac{1}{2} \mathbf{u}^\top (z^p \mathbf{K}) \mathbf{u} + R(z) \\ \text{s.t.} \quad & (z^p \mathbf{K}) \mathbf{u} - f = 0 \\ & \frac{V(z)}{V_o} \leq \gamma \end{aligned}$$

Nonlinear Programming Solver's

Formulation

$$\begin{aligned} & \min \quad \frac{1}{2} \mathbf{u}^\top (z^p \mathbf{K}) \mathbf{u} + R(z) + \frac{1}{2} (V(z) - \gamma V_o)^2 \\ \text{s.t.} \quad & (z^p \mathbf{K}) \mathbf{u} - f = 0 \end{aligned}$$

Test Problems



Mitchell



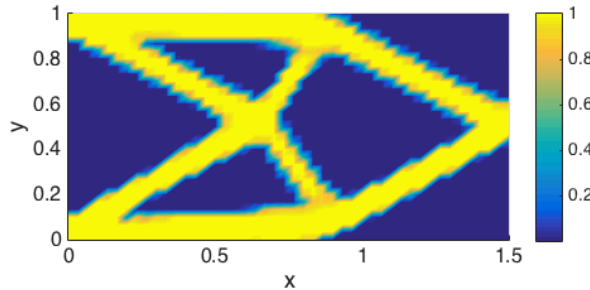
Cantilever



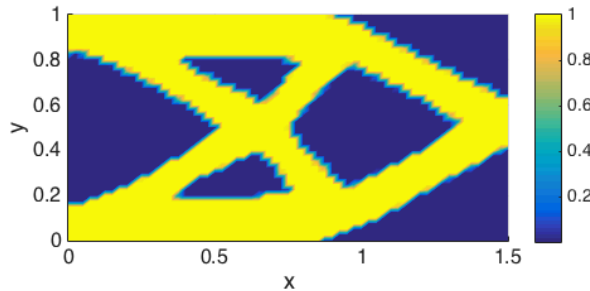
MBB

Example 1: 60x40 FE Mesh

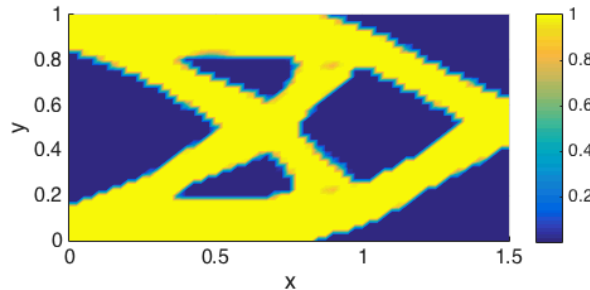
OC



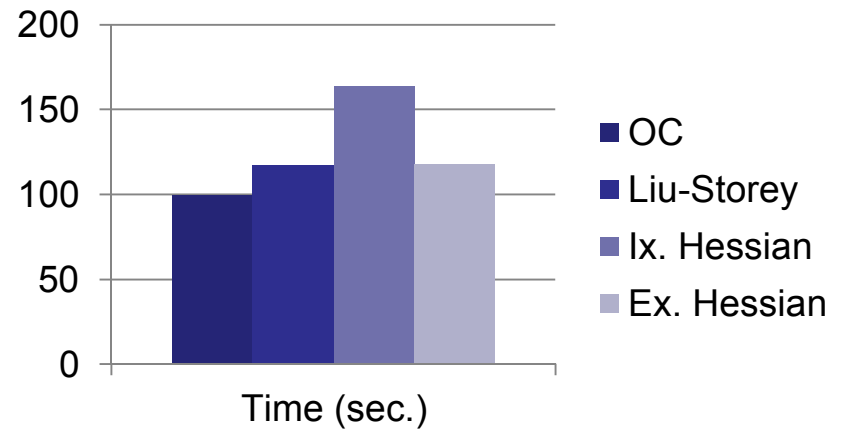
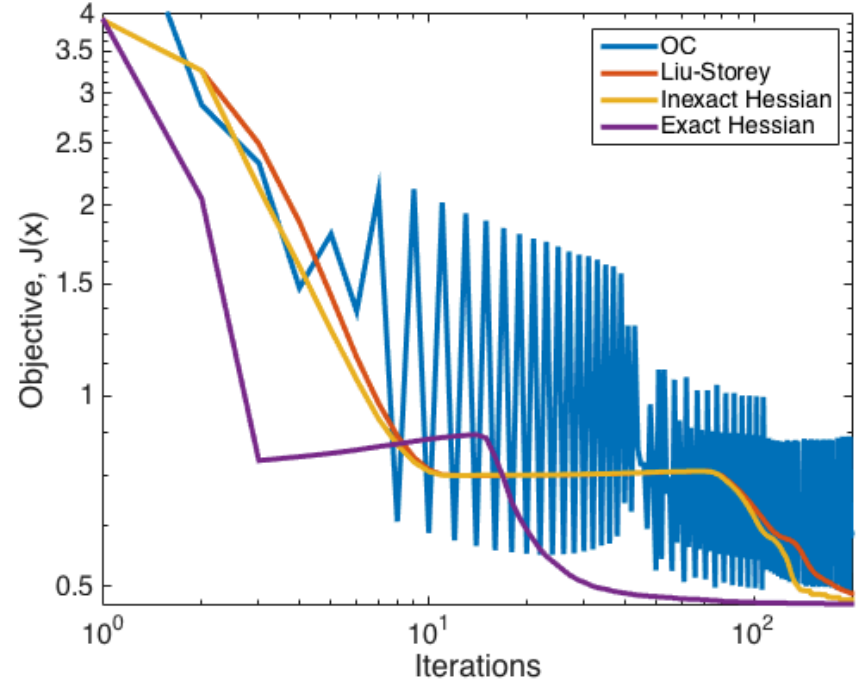
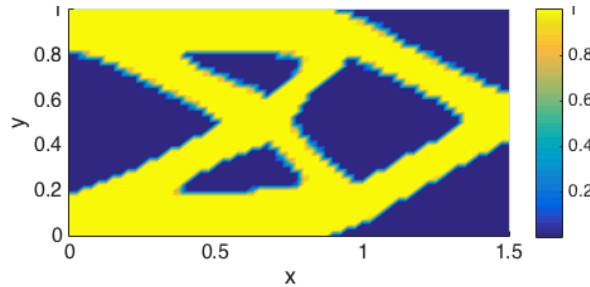
Liu-Storey



Ix. Hessian

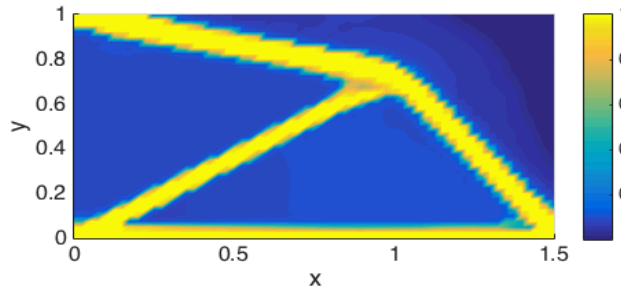


Ex. Hessian

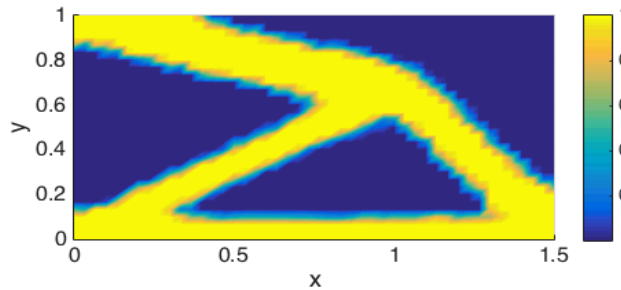


Example 2: 60x40 FE Mesh

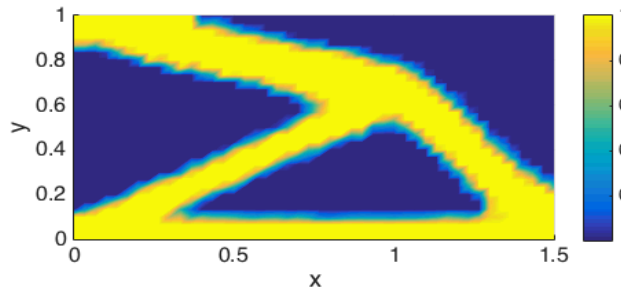
OC



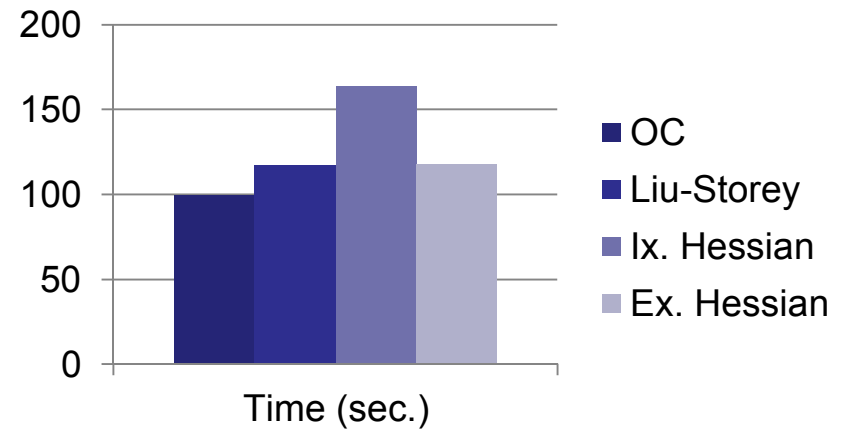
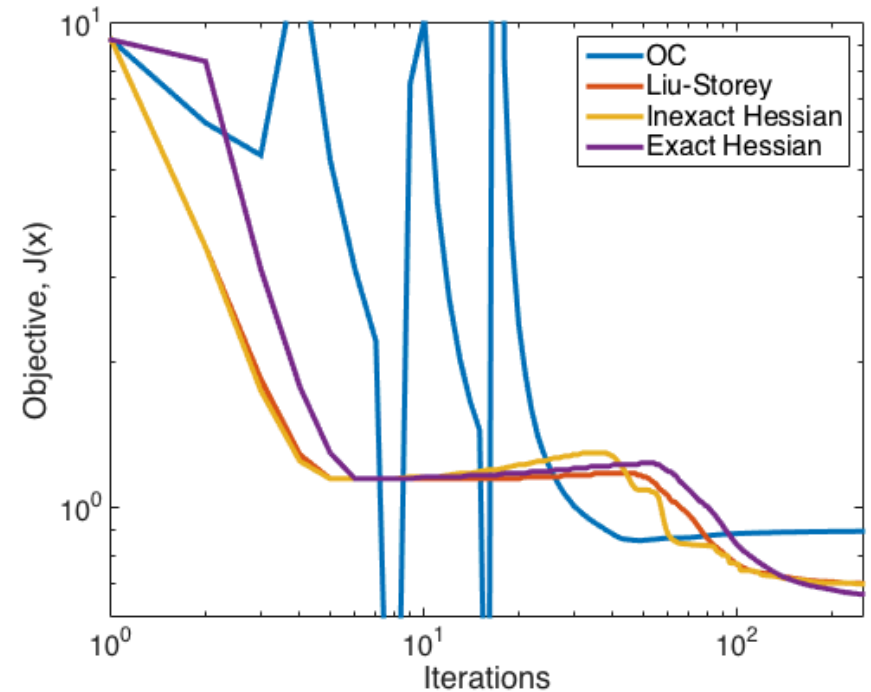
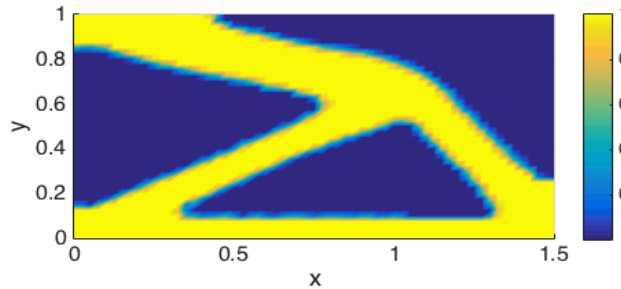
Liu-Storey



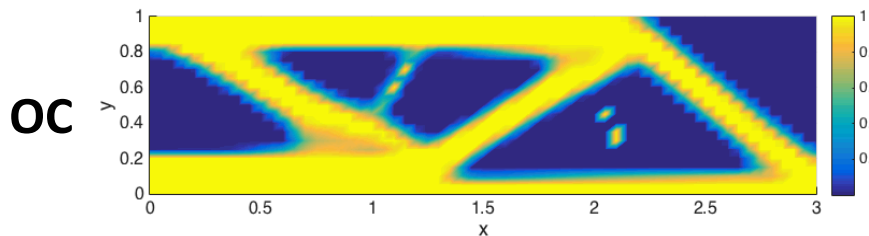
Ix. Hessian



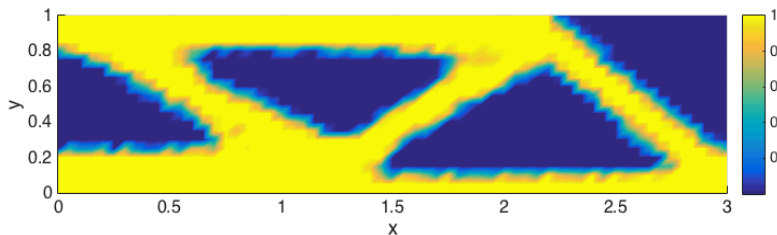
Ex. Hessian



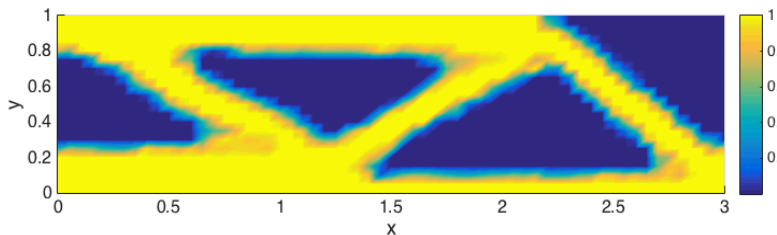
Example 3 (60x20)



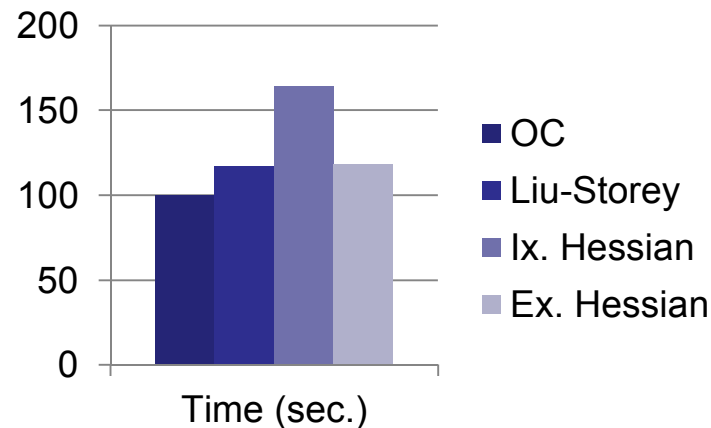
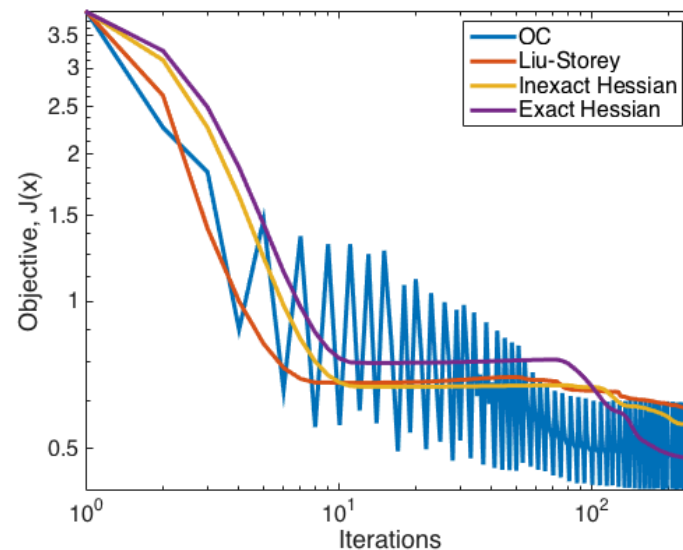
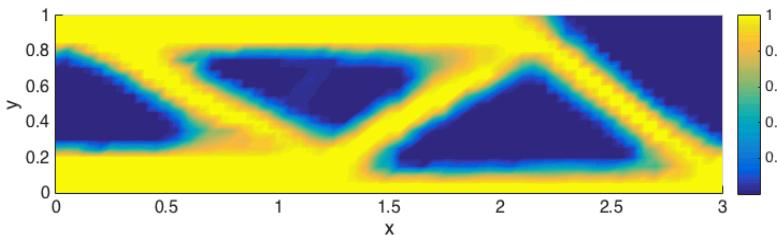
Liu-Storey



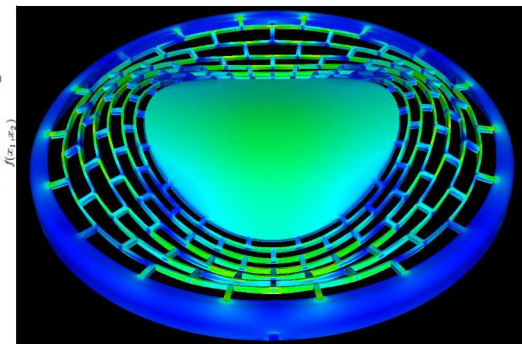
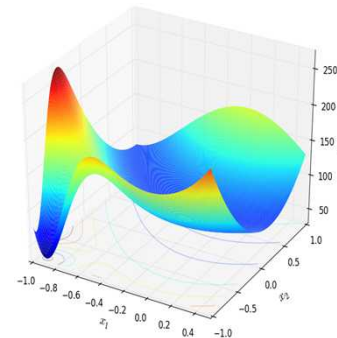
Ix. Hessian



Ex. Hessian



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Future Research Directions



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Final Remarks

- **Additional tasks**

- Compare performance against MMA and GCMMA algorithms
- Exercise formulation based on filters and stress minimization problems

- **Algorithmic Improvements**

- Research in primal-dual interior-point methods
- Explore task parallelism of solves needed for inexact Hessian computation
- Reduced order model based optimization algorithm
 - Allow optimization algorithm to automatically generate and update reduced order model for physics