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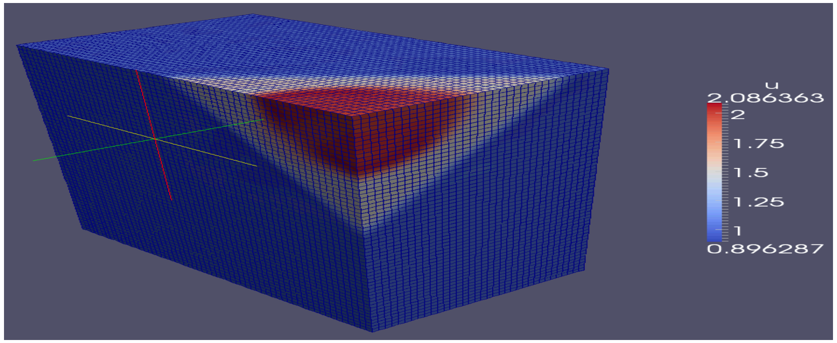

Application of Second-Order Optimization Algorithms to Topology Optimization Problems

July 24, 2014

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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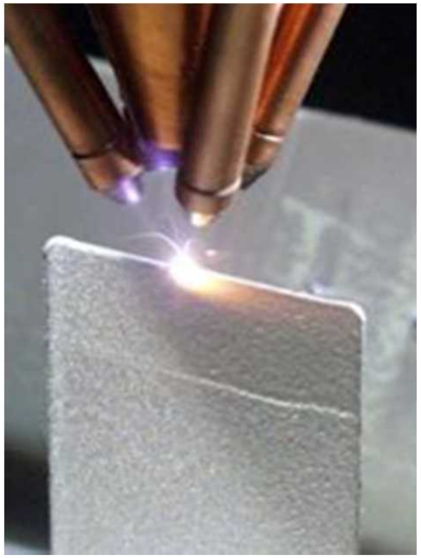
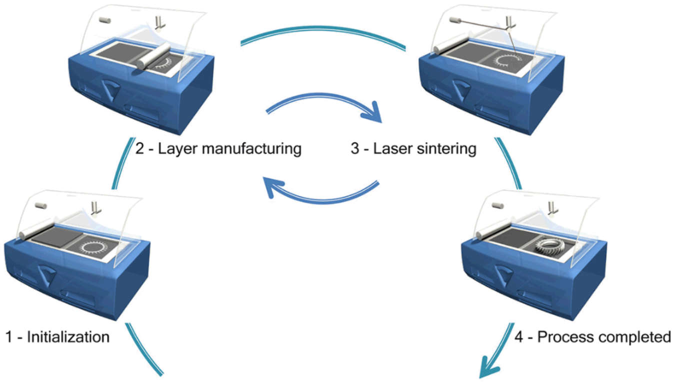
Agenda

- Motivation
- Linear Programming vs. Nonlinear Programming
- Full-Space & Reduced-Space Formulations
- Optimization Framework
- Design Optimization Toolkit (DOTk)
- Example Problem
- Future Directions
- Summary

Additive Manufacturing (AM)



LENS® deposition process



Phenix™ Systems powder bed process

Advantages

1. Eliminates conventional manufacturing restrictions
2. Expands design space
3. Opportunity to engineer geometries and materials to satisfy intended function
4. Rapid prototyping

Needs & Opportunities (Bourell, D.L. et al.)

1. Design
2. Process modeling & control
3. Material processes & machines
4. Biomedical applications
5. Energy & sustainability applications

Topology Optimization

Problem Definition

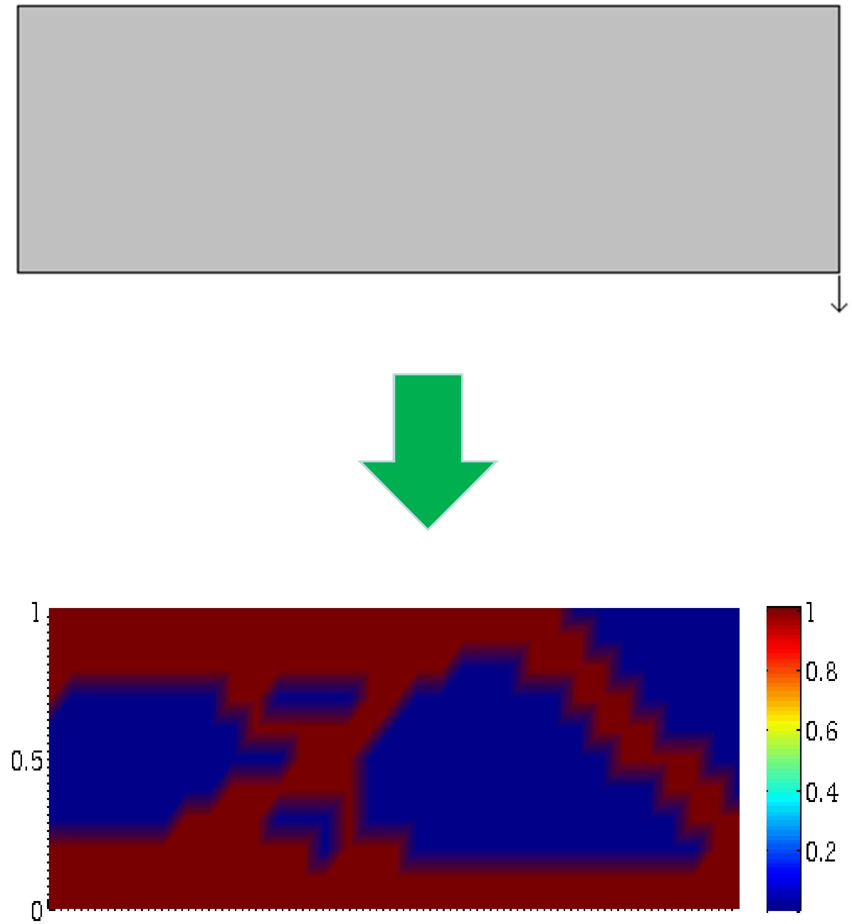
Let Z and Y denote Banach spaces where $z \sim z \ \forall \ z \in Z$. Lets also define an objective function and equality constraint of the form $J\colon Z \rightarrow \mathbb{R}$ and $g\colon Z \rightarrow Y$. This leads to a linear programming problem of the form:

$$\min_{z \in Z} J(z) \quad s.t. \ \ g(z) = 0$$

where $Z = \{z \mid a \leq z \leq b\}$.

Derivative Operators

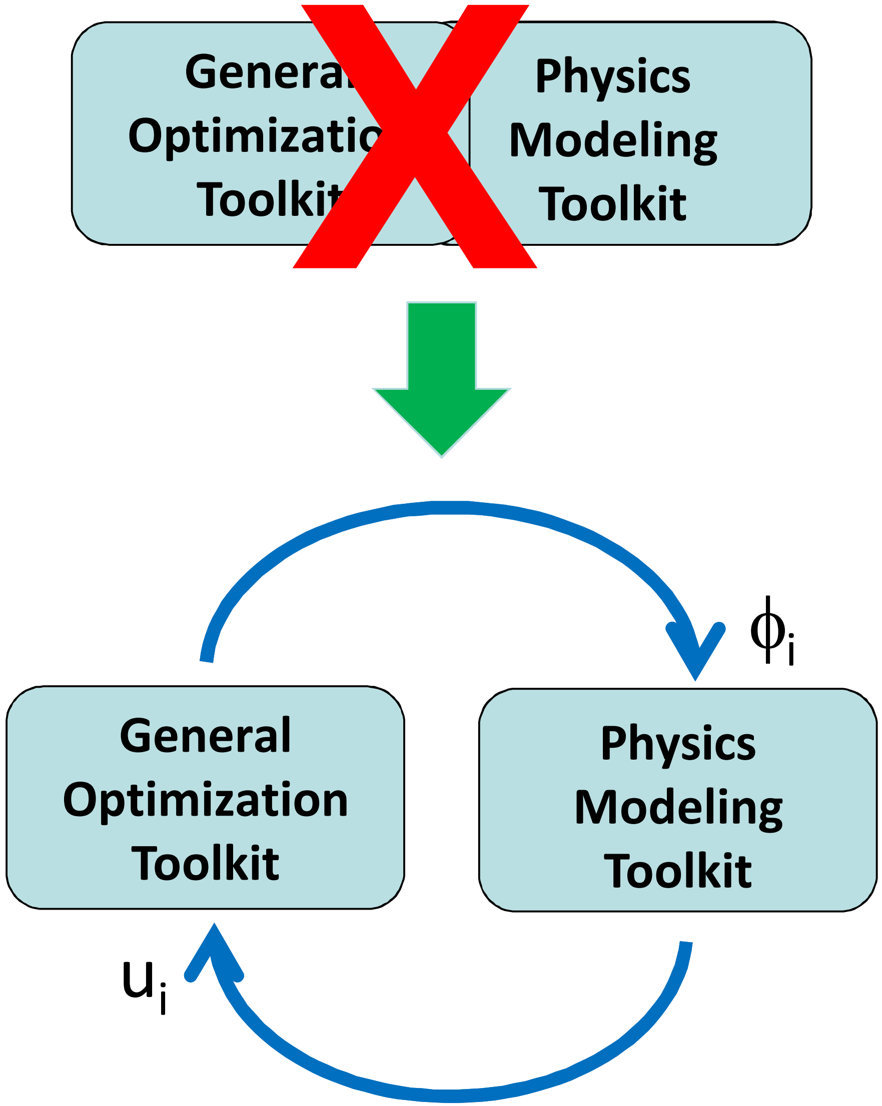
$J_z, J_{zz}, (g_z)^*, (g_{zz})^*$



Topology Optimization Timeline

Foundational Work

1. Method of moving asymptotes introduced (Svanberg, K.)
2. Homogenization method introduced (Bendsøe, M. et al.)
3. Structural design via optimality criteria (Rozvany, G.)
4. Numerical instabilities in topology optimization (Sigmund, O. et al.)
5. Krylov subspace methods with recycling (Wang, S. et al.)
6. Topology optimization survey (Sigmund, O. et al.)



Linear Programming (LP) Method

LP Formulation

$$\min_{z \in Z} J(z) \;\; s.t. \;\; g(z) = 0$$

Advantages

1. Second-order formulation: Four derivative operators required, $J_z, \;\; J_{zz}, g_z, g_{zz}$
   a. First-order formulation: Two derivative operators are usually derived and implemented, J_z and g_z
2. Equality constraint derivative operators are not reassembled at each iteration
3. Ease of implementation

Simplification

Apply optimality criteria (OC) approach (Rozvany, 1989)

$$\min_{z \in Z} J(z)$$

Advantages

1. Only $J(z)$ first- and second-order derivative operators are used
2. $g(z)$ first- and second-order derivative operators are not required
3. Ease of implementation

LP Method Cont.

Disadvantages

Unconstraint:

$$\min_{z \in Z} J(z)$$

yields accurate first- and second-order derivative operators but inaccurate problem formulation is solved

Why? Nonlinear programming method require to properly solve optimization problem

Equality Constraint:

$$\min_{z \in Z} J(z) \;\; s.t. \;\; g(z) = 0$$

leads to inaccurate first- and second-order derivative operators.

Why? Let U denote a Banach space | $u \sim u \; \forall \; u \in U$. Then, $g: U \text{ x } Z \rightarrow Y$ and $u(z): Z \rightarrow U$

Nonlinear Programming Method

Problem Definition

Let U, Z, and Y denote Banach spaces where $u \sim u \; \forall \; u \in U$, $z \sim z \; \forall \; z \in Z$. Lets also define an objective function and equality constraint of the form $J: U \text{ x } Z \rightarrow \mathbb{R}$ and $g: U \text{ x } Z \rightarrow Y$. This leads to a nonlinear programming problem (NLP) of the form:

$$\min_{(u,z) \in U \text{x} Z} J(u,z) \;\; s.t. \;\; g(u,z) = 0$$

where $Z = \{z \mid a \leq z \leq b\}$.

Lagrangian functional

Let $L(u,z,y): U \text{ x } Z \text{ x } Y \rightarrow \mathbb{R}$ be defined as $L(u,z,y) = J(u,z) + \langle y, g(u,z) \rangle_{Y^*,Y}$, where $Y^*: Y \rightarrow U \text{ x } Z$ and $\langle \cdot,\cdot \rangle: X \text{ x } X \rightarrow \mathbb{R}$ denotes the inner product for a given Banach space X.

Solution Strategy: Full-Space

Full-Space Formulation

1. Derive first-order necessary optimality conditions (FONOC)
2. Apply Newton's method to FONOC
3. Solve Karush-Kuhn-Tucker (KKT) optimality system $\nabla^2 L(u,z,y) = -\nabla L(u,z,y)$, where[1]

$$\begin{pmatrix} L_{uu} & L_{uz} & (g_u)^* \\ L_{zu} & L_{zz} & (g_z)^* \\ g_u & g_z & 0 \end{pmatrix} \begin{pmatrix} \delta u \\ \delta z \\ \delta y \end{pmatrix} = - \begin{pmatrix} J_u + \langle (g_u)^*, y \rangle_{Y^*,Y} \\ J_z + \langle (g_z)^*, y \rangle_{Y^*,Y} \\ g \end{pmatrix}$$

Here,

$$L_{uu} = J_{uu} + \langle (g_{uu})^*, y \rangle_{Y^*,Y} \quad L_{uz} = J_{uz} + \langle (g_{uz})^*, y \rangle_{Y^*,Y}$$

$$L_{zu} = J_{zu} + \langle (g_{zu})^*, y \rangle_{Y^*,Y} \quad L_{zz} = J_{zz} + \langle (g_{zz})^*, y \rangle_{Y^*,Y}$$

1. *Operators dependency on (u, z, y) drop for simplicity*

Solution Strategy: Reduced-Space

Reduced-Space Formulation

The implicit function (Danilov, V.) theorem admits the definition of a solution operator $\hat{u}: Z \to U$ such that $\{(\hat{u}(z), z) \mid z \in Z\} = \{(u, z) \in U \text{ x } Z \mid g(u, z) = 0\}$. This allows to redefine the optimization problem as

$$\min_{z \in Z} J(\hat{u}(z), z)$$

Solution Strategy (First-order information)

1. Solve $g(\hat{u}(z), z) = 0$ for $\hat{u}(z) \in U$
2. Solve $g_u(\hat{u}(z), z)^* y = -J_u(\hat{u}(z), z)$ for $y \in Y$
3. Compute reduced gradient operator

$$\nabla J(\hat{u}(z), z) = J_z(\hat{u}(z), z)^* + \langle g_u(\hat{u}(z), z)^*, y \rangle_{Y^*, Y}$$

Solution Strategy: Reduced-Space

Solution Strategy (Second-order information)

4. Solve $g_u(\hat{u}(z), z)\delta u = -g_z(\hat{u}(z), z)\delta z$ for $\delta u \in U$, where $\delta z \in Z$ denotes the trial step
5. Solve $g_u(\hat{u}(z), z)^* \delta y = -[L_{uu}(\hat{u}(z), z, y)\delta u + L_{uz}(\hat{u}(z), z, y)\delta z]$ for $\delta y \in Y$
6. Compute application of reduced Hessian operator to δz

$$\nabla^2 J(\hat{u}(z), z) = L_{zu}(\hat{u}(z), z, y)\delta u + L_{zz}(\hat{u}(z), z, y)\delta z + L_{zy}(\hat{u}(z), z, y)\delta y$$

Notes

- Step 1-3 are applied for first-order methods
- Step 1-6 are applied for second-order methods

Common Elements

Both full- and reduced-space formulation strategies required the same set of operators to solve a given optimization problem.

Objective Function Operators

$J(u,z),\ J_u(u,z),\ J_z(u,z),\ J_{uu}(u,z),\ J_{uz}(u,z),\ J_{zz}(u,z),\ J_{zu}(u,z)$

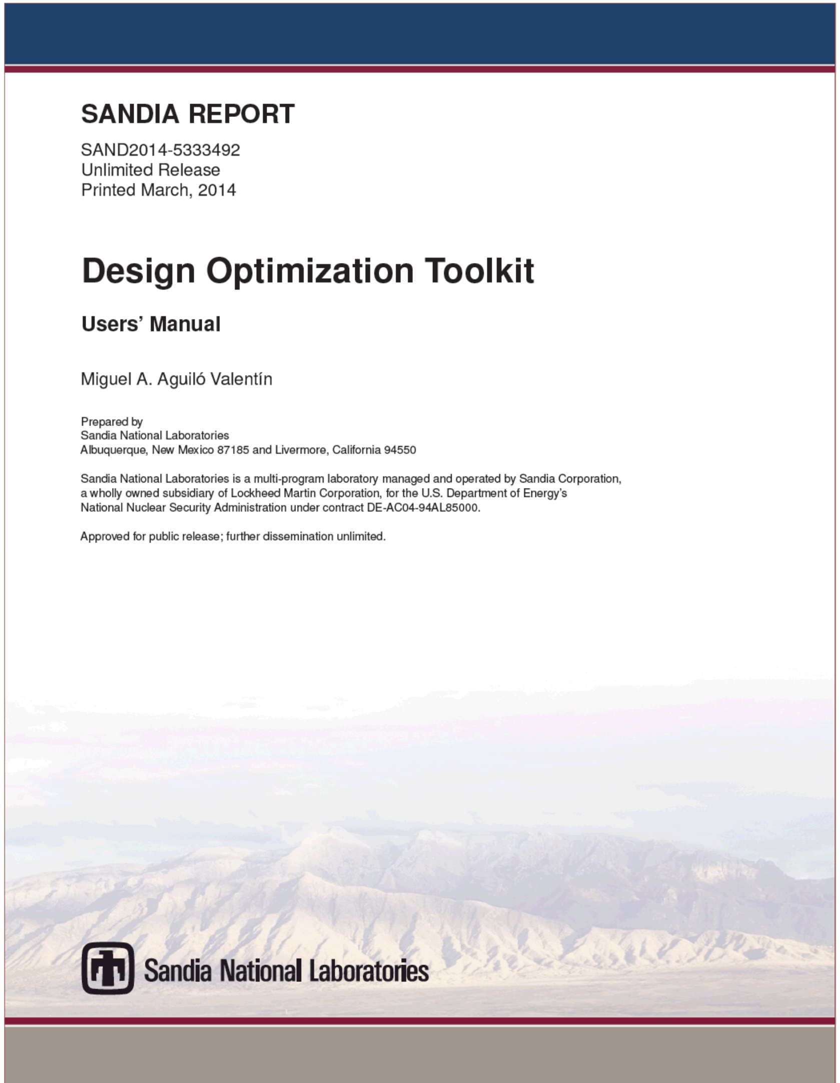
Equality Constraint Operators

$$g(u,z),\ g_u(u,z),\ g_u(u,z)^*, g_z(u,z), g_z(u,z)^*,$$
$$g_{uu}(u,z)^*, g_{uz}(u,z)^*, g_{zz}(u,z)^*, g_{zu}(u,z)^*$$

Note

Additional operators may be required for certain classes of inequality constraints.

Design Optimization Toolkit (DOTk)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Design Optimization Toolkit

Users' Manual

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- Stand-alone C++ software package
- Range of solution methods for general gradient- and nongradient-based constrained optimization
  - Nonlinear CG, line search quasi-Newton, trust region quasi-Newton, line search Newton CG, trust region Newton CG, trust region inexact SQP
  - Matrix-free
- Other tools include
  - *In situ* solvers
  - *In situ* preconditioners
  - *In situ* derivative operators diagnostics tools
- MATLAB API to enable direct used of DOTk solution methods through MATLAB
  - Python API in progress

Application Programming Interface

Linear Algebra API

$$scal(\alpha, x): \alpha x \to x$$

$$axpy(\alpha, x, y): \alpha x + y \to y$$

$$innr(x, y): x^T y \to \mathbb{R}$$

$$normF(A): \sqrt{tr(A^T A)} \to \mathbb{R}$$

Operators API

$$F(u, z) \equiv F: UxZ \to \mathbb{R}$$

$$F_u(u, z, output) \equiv F_u: UxZ \to output$$

$$F_z(u, z, output) \equiv F_z: UxZ \to output$$

$$F_{uu}(u, z, du, output) \equiv F_{uu}: UxZx\widehat{U} \to output$$

$$F_{uz}(u, z, dz, output) \equiv F_{uz}: UxZx\hat{Z} \to output$$

$$F_{zz}(u, z, dz, output) \equiv F_{zz}: UxZx\hat{Z} \to output$$

$$F_{zu}(u, z, du, output) \equiv F_{zu}: UxZx\widehat{U} \to output$$

$$G(u, z, output) \equiv G: UxZ \to output$$

$$G_u(u, z, du, output) \equiv G_u: UxZx\overline{U} \to output$$

$$G_z(u, z, dz, output) \equiv G_z: UxZx\bar{Z} \to output$$

$$G_u(u, z, y, output)^* \equiv G_u: UxZxY \to output$$

$$G_z(u, z, y, output)^* \equiv G_z: UxZxY \to output$$

$$G_{uu}(u, z, y, du, output)^* \equiv G_{uu}: UxZxYx\widehat{U} \to output$$

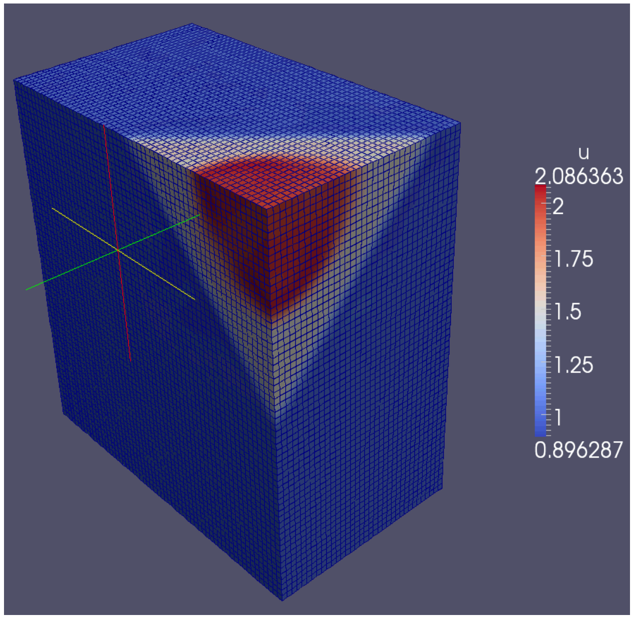
$$G_{uz}(u, z, y, dz, output)^* \equiv G_{uz}: UxZxYx\hat{Z} \to output$$

$$G_{zz}(u, z, y, dz, output)^* \equiv G_{zz}: UxZxYx\hat{Z} \to output$$

$$G_{zu}(u, z, y, du, output)^* \equiv G_{zu}: UxZxYx\widehat{U} \to output$$

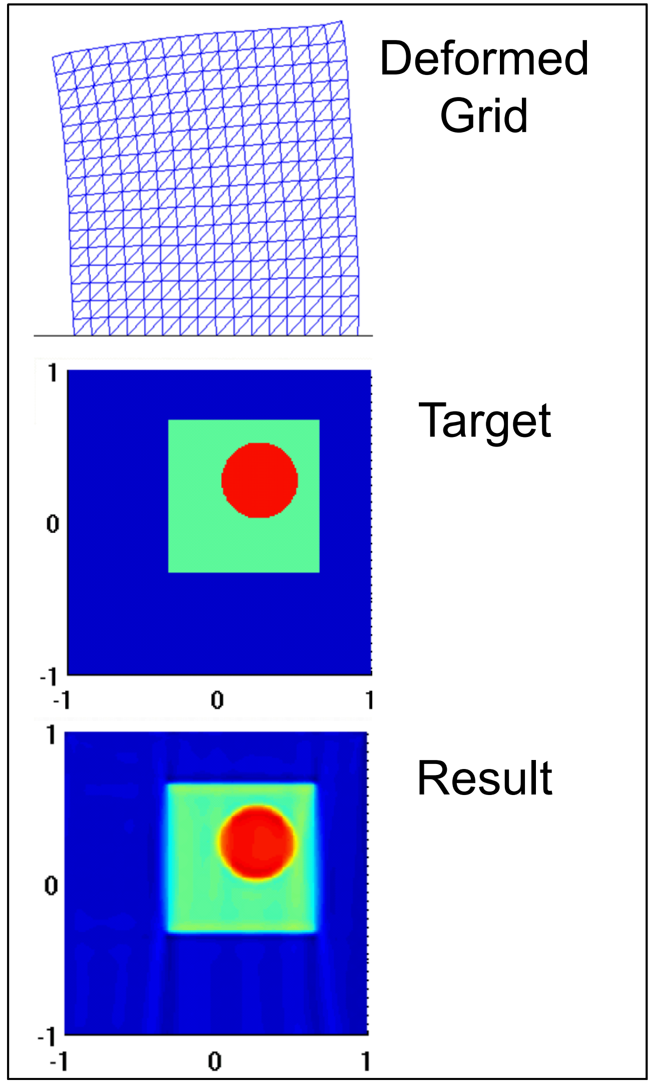
Endless Possibilities

Large-Scale Optimization

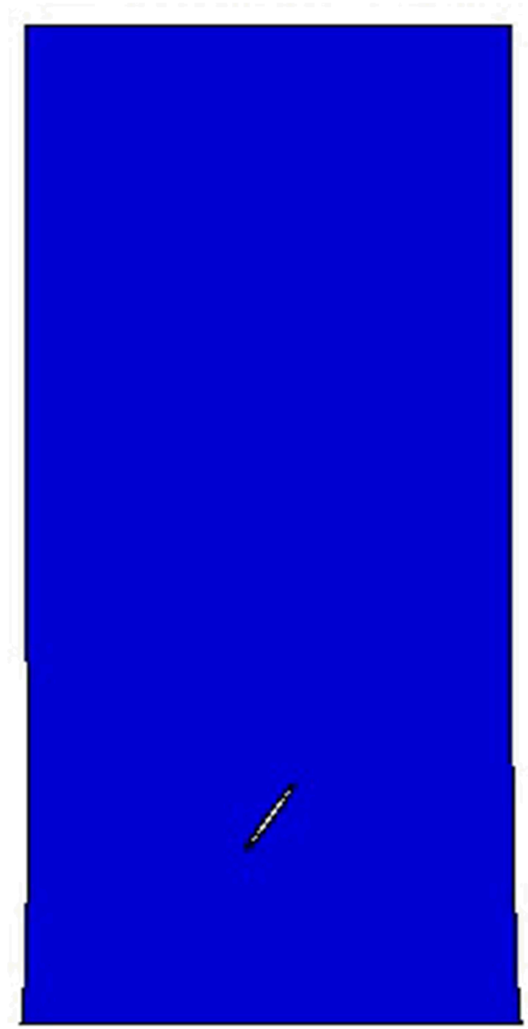


Topology Optimization

Inverse Problems



Crack Identification



Example: Topology Optimization

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Problem Definition

A topology optimization problem is often formulated as

$$\min_{(u,z)\in U\text{x}Z} J(u,z)$$
$$\text{s.t.}$$
$$g(u,z)=0$$
$$V(z)\le \gamma V_0$$

were $Z=\{z \mid a\le z\le b\}$.

Alternate Definition

The above topology optimization problem can be formulated as

$$\min_{(u,z)\in U\text{x}Z} J(u,z)+(V(z)-\gamma V_0)^2$$
$$\text{s.t.}$$
$$g(u,z)=0$$

were $Z=\{z \mid a\le z\le b\}$.

Density Field Definition

Lets define Lebesgue space $Z\equiv L^2(\Omega,\mathbb{R})$ of square measurable C^0-functions endowed with inner product

$$\langle z,z\rangle_Z=\int_\Omega z\,z \quad \text{for } z\in Z$$

and norm $\|z\|_Z=(\langle z,z\rangle_Z)^{1/2}$.

Alternate Definition

Lets define Lebesgue space $\hat{Z}\equiv Z^1(\Omega,\mathbb{R})$ of square measurable C^1-functions endowed with inner product

$$\langle z,z\rangle_{\hat{Z}}=\langle z,z\rangle_Z+\sum_{i=1}^{\dim(\Omega)}\langle z_{,i},z_{,i}\rangle_Z$$

and norm $\|z\|_{\hat{Z}}=(\langle z,z\rangle_{\hat{Z}})^{1/2}$.

Case Study

Equality Constraint

$$-\left(\boldsymbol{C}_{ijkl}\epsilon_{kl}\right)_{,j} = 0 \text{ in } \Omega$$
$$u_i = 0 \text{ on } \partial\Omega_u$$
$$\left(\boldsymbol{C}_{ijkl}\epsilon_{kl}\right)n_j = \tau_i \text{ on } \partial\Omega_\tau$$

Objective Function

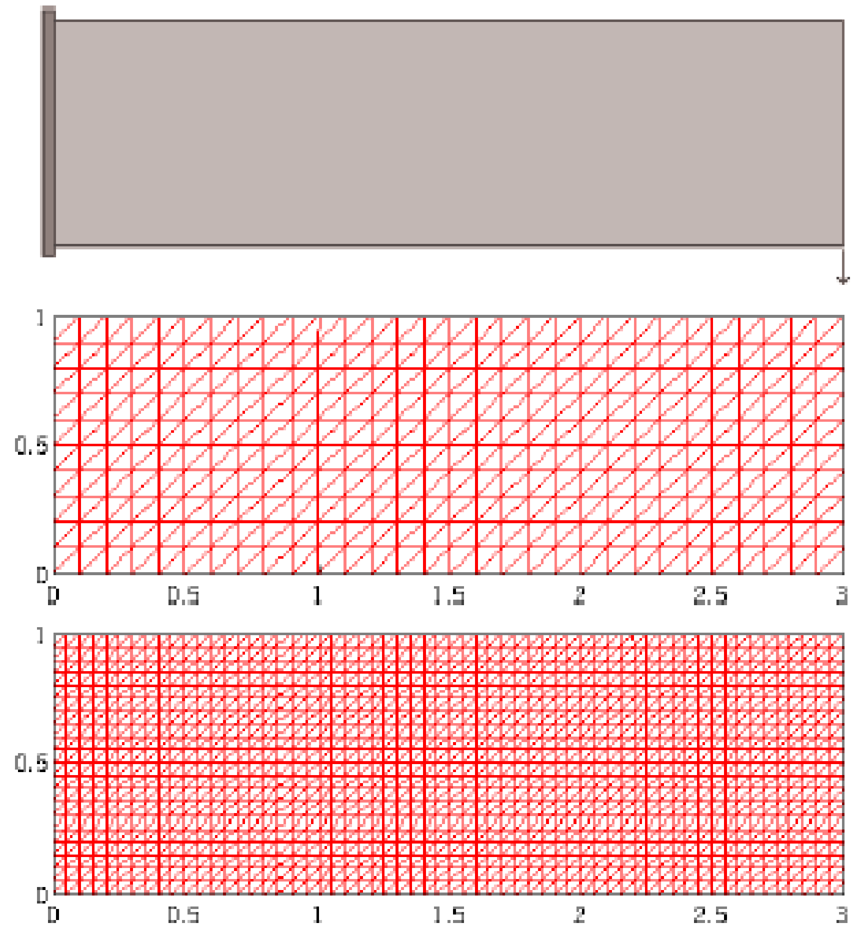
$$J(u_i, z) = \frac{\beta}{2}\left\langle D(z)\boldsymbol{C}_{ijkl}\epsilon_{kl}, \epsilon_{ij}\right\rangle + V(z)$$

<u>Volume Term</u>:

$$V(z) = \frac{\alpha}{2}\left(\sum_{e=1}^{N_e} V_e z - \gamma V_0\right)^2$$

<u>Density Model</u>:

$$D(z) = E_{min} + z^p(E_0 - E_{min})$$



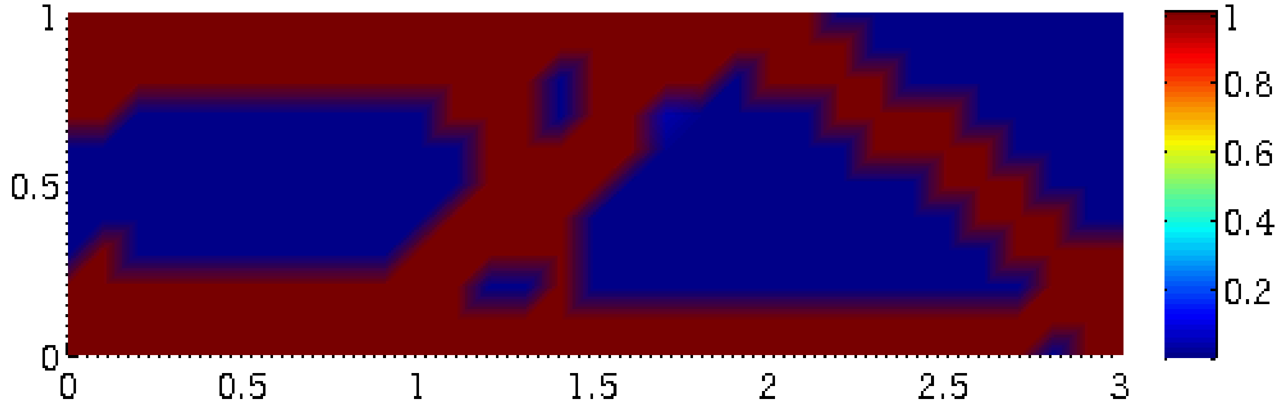
Results

Notes:

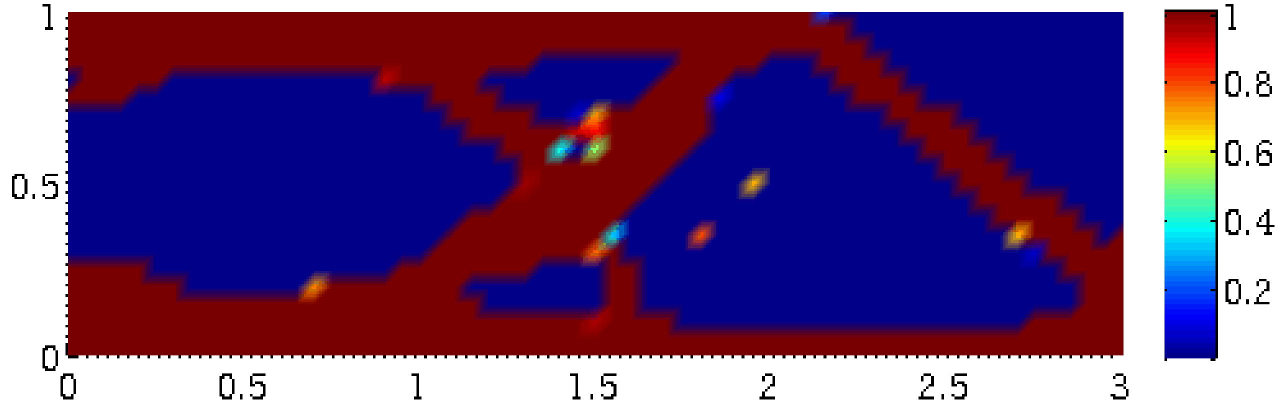
1. Trust region Newton CG algorithm
2. 210 Iterations needed to reach optimal solution, i.e. $\|\delta z\| < 1\text{x}10^{-18}$ and $\|\nabla J\| < 1\text{x}10^{-12}$
3. Filtering operator was not used

Results: Nonlinear CG

30x10 FEM Grid

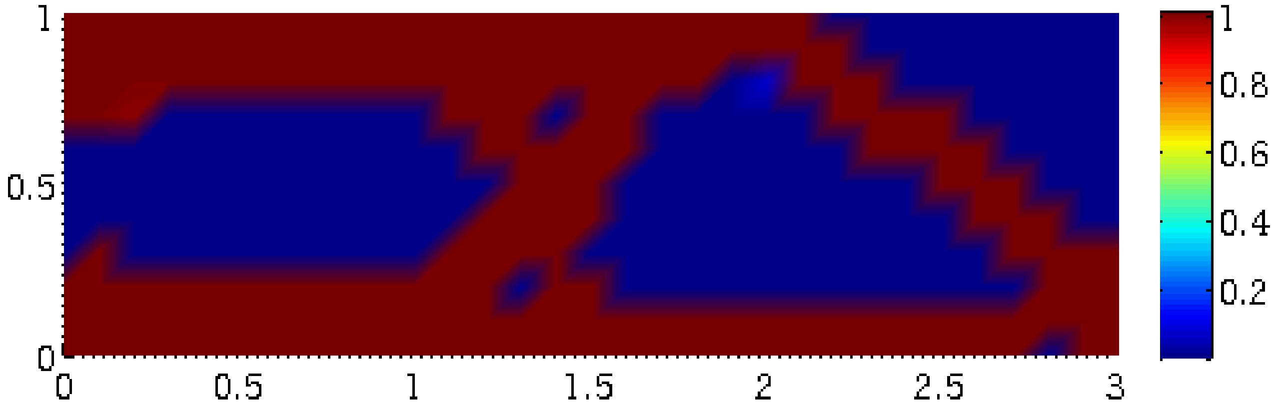


60x20 FEM Grid

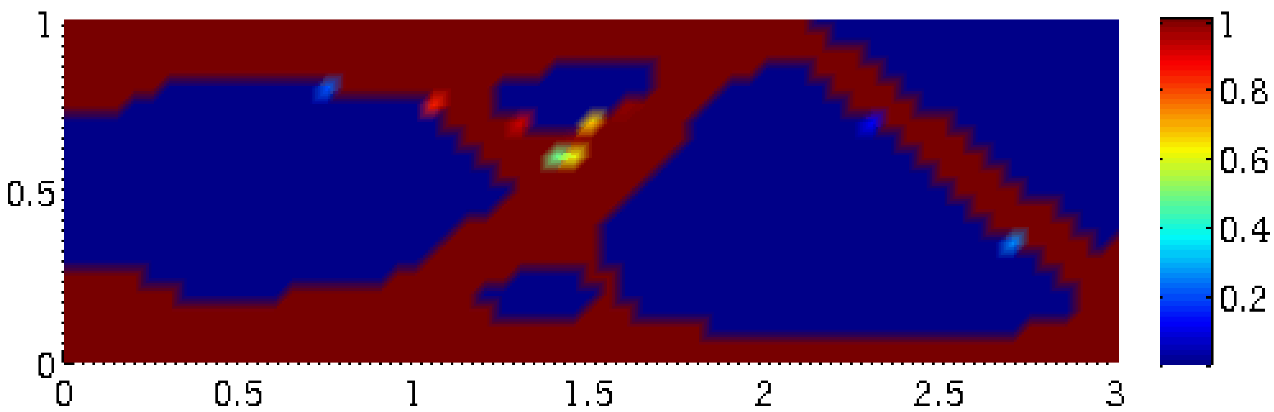


Results: Line Search Newton CG

30x10 FEM Grid

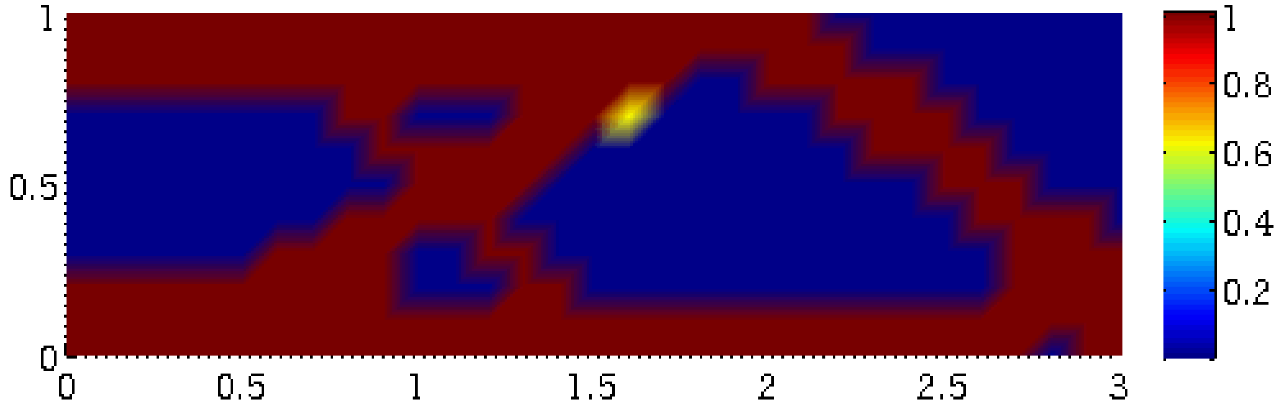


60x20 FEM Grid

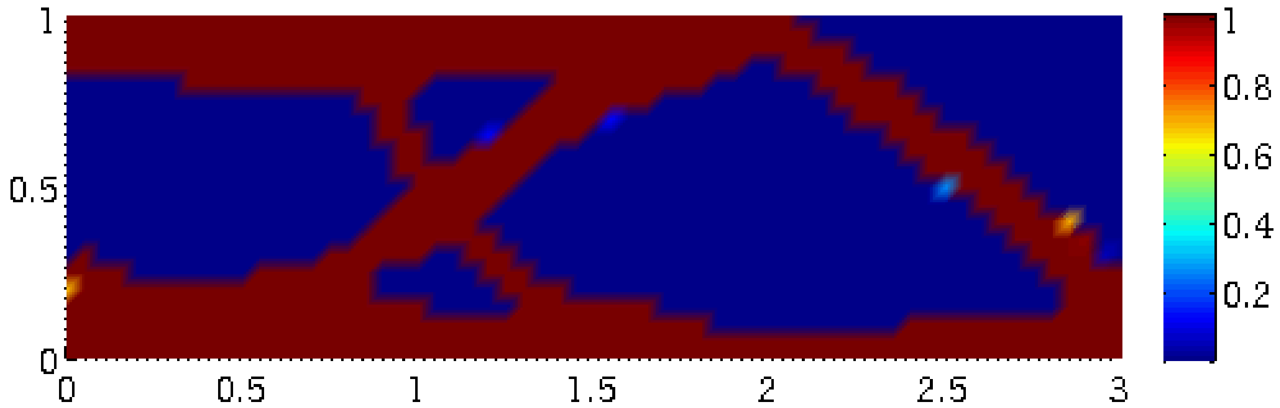


Results: Trust Region Newton CG

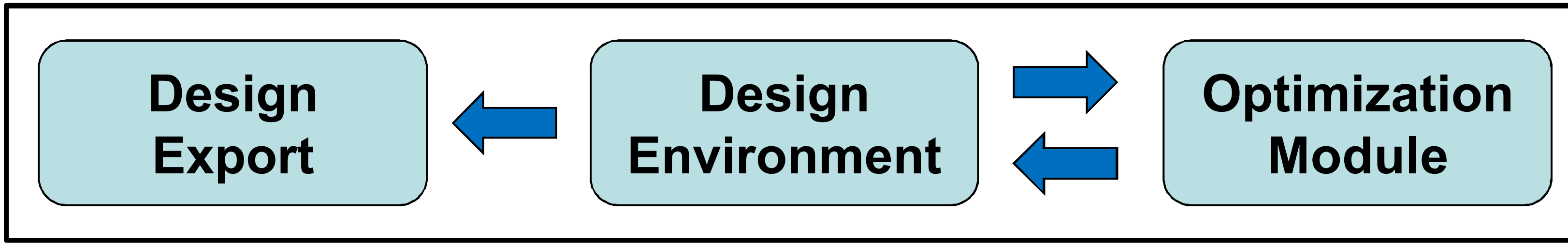
30x10 FEM Grid

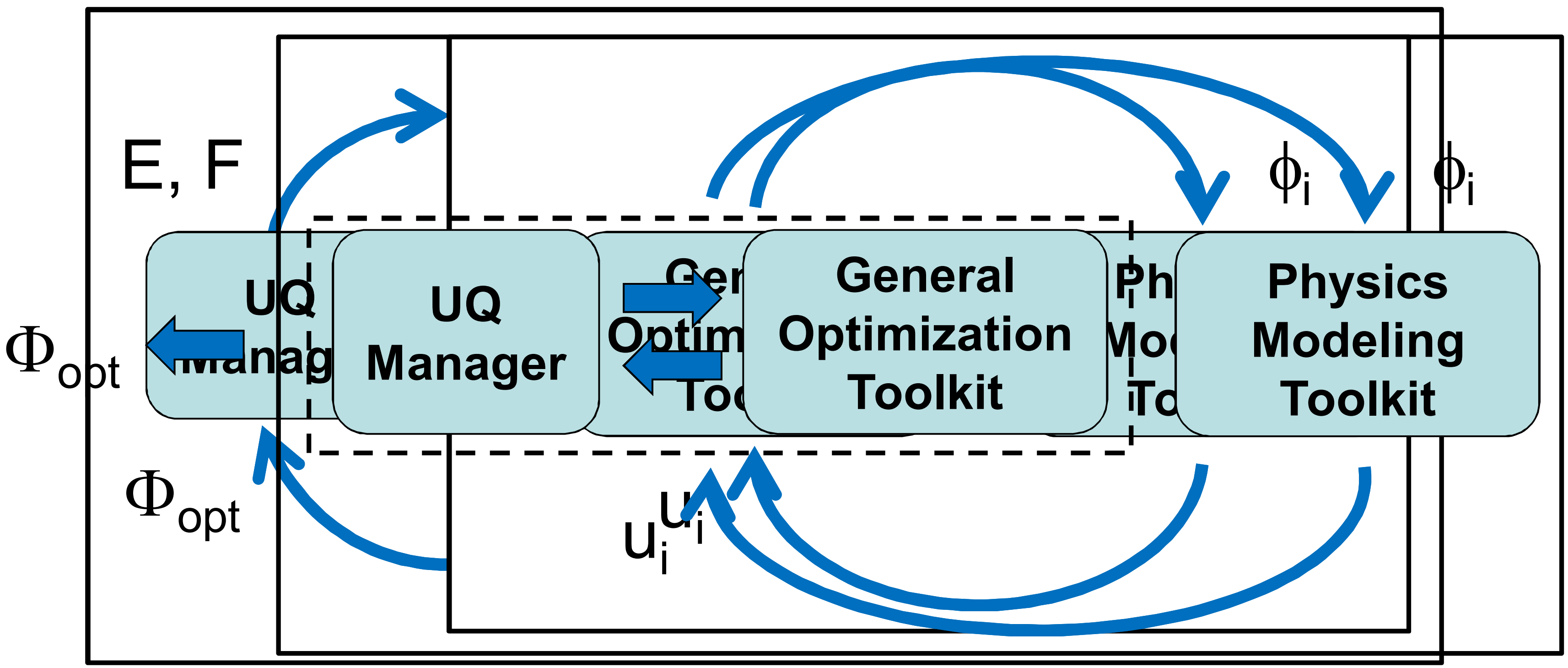


60x20 FEM Grid



The Vision


Design Export
Design Environment
Optimization Module


E, F
UQ Manager
General Optimization Toolkit
Physics Modeling Toolkit
Φ_{opt}
Φ_{opt}
ϕ_i
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Further Advances

Precise Embedding of Uncertainty into the Topology Optimization Problem

To directly incorporate the notion of uncertainty into the mathematical formulation of the topology optimization problem we require

- ***Research***: Advances in algorithmic research such as new parallel optimization algorithms, formulation strategies, faster sampling algorithms, parallel solvers, preconditioners, numerical methods for stochastic topology optimization, and more
- ***Numerical Tool***: Proper implementation of the advances in algorithmic research into a common optimization library suited for general constrained optimization problems

DOTk

Final Remarks

For constrained topology optimization problems:

- Optimization framework enables separation of physics modeling software packages from the optimization library
- Alternate topology optimization formulation was successfully applied
- General-purpose optimization algorithms can be successfully applied to solve topology optimization problems
- Filtering operator was not needed in the present case study
- Research in interior-point methods is required for accurate modeling of general constraints

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