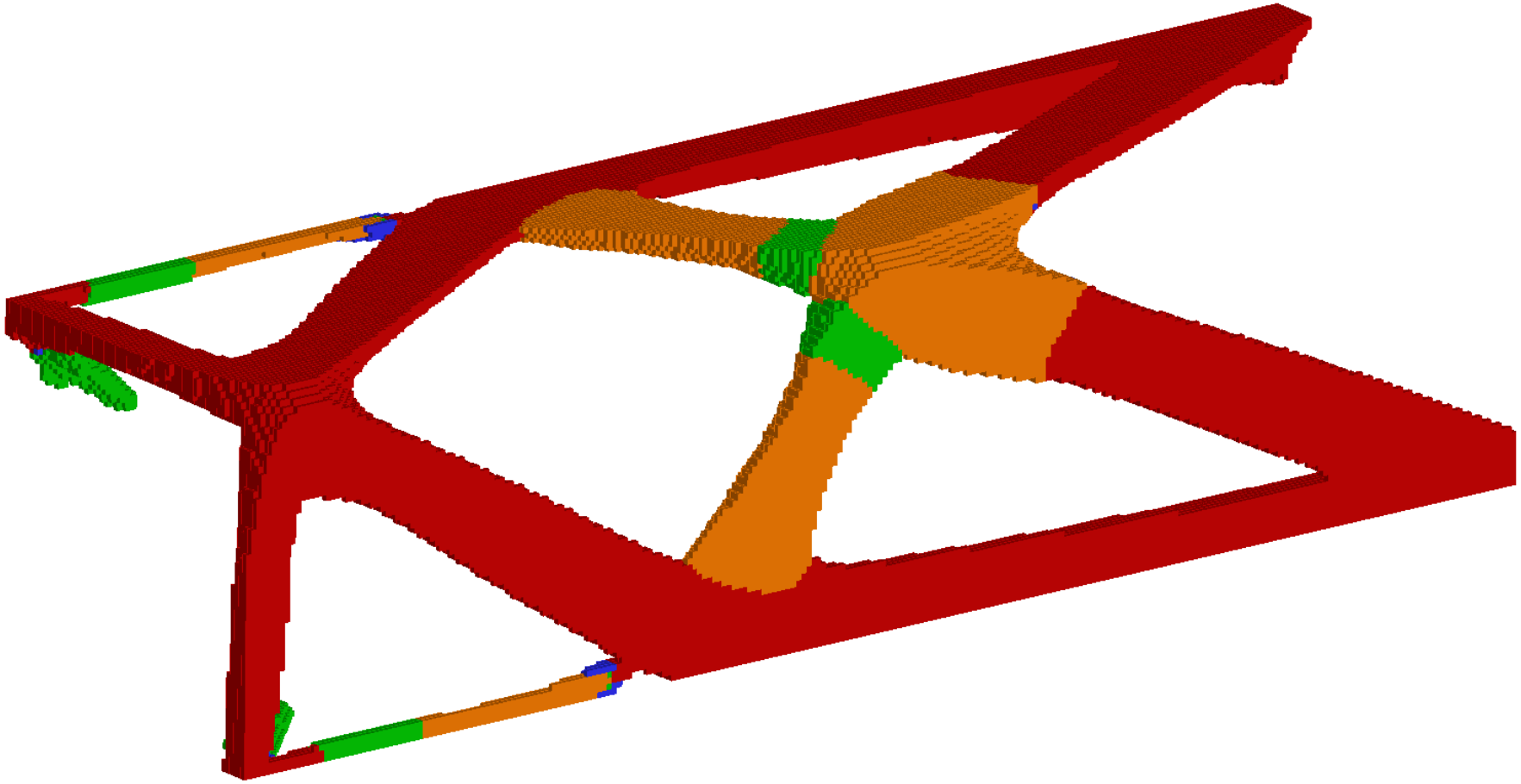
Large-Scale Topology Optimization Methods for Additively Manufactured Structures

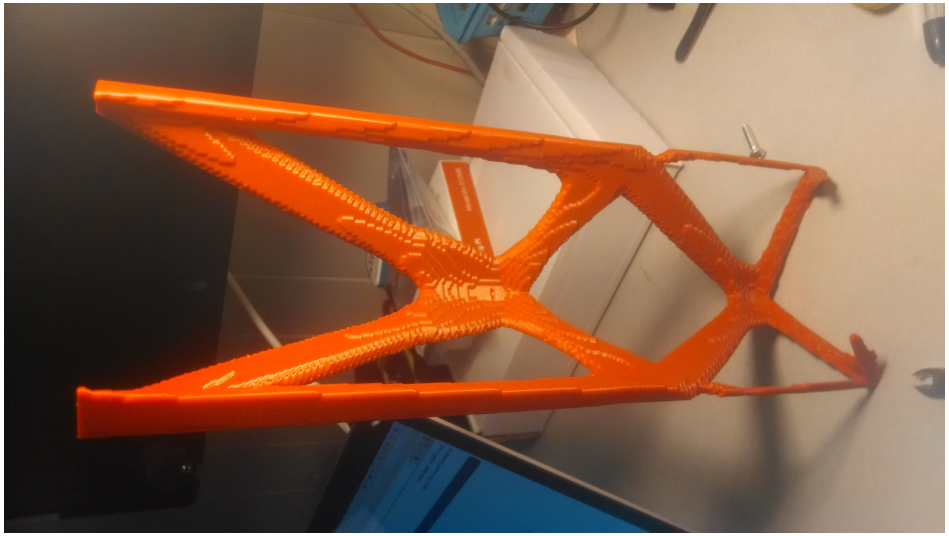


Graeme J. Kennedy, Georgia Tech

Additive manufacturing technologies

- Greatly reduce or remove geometric restrictions
- Multimaterial manufacturing methods enable additional structural tailoring
- Metallic additive manufacturing for primary structures?

Polymer-based single material



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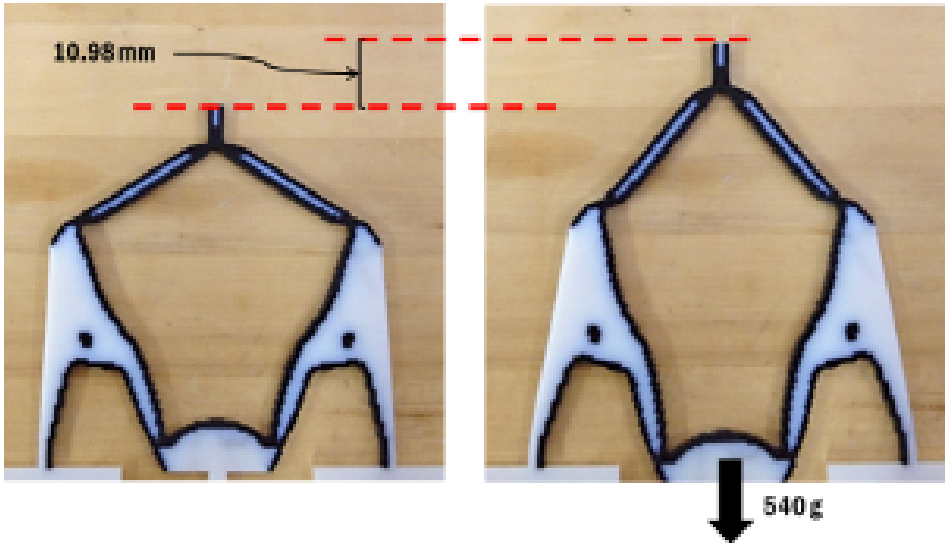
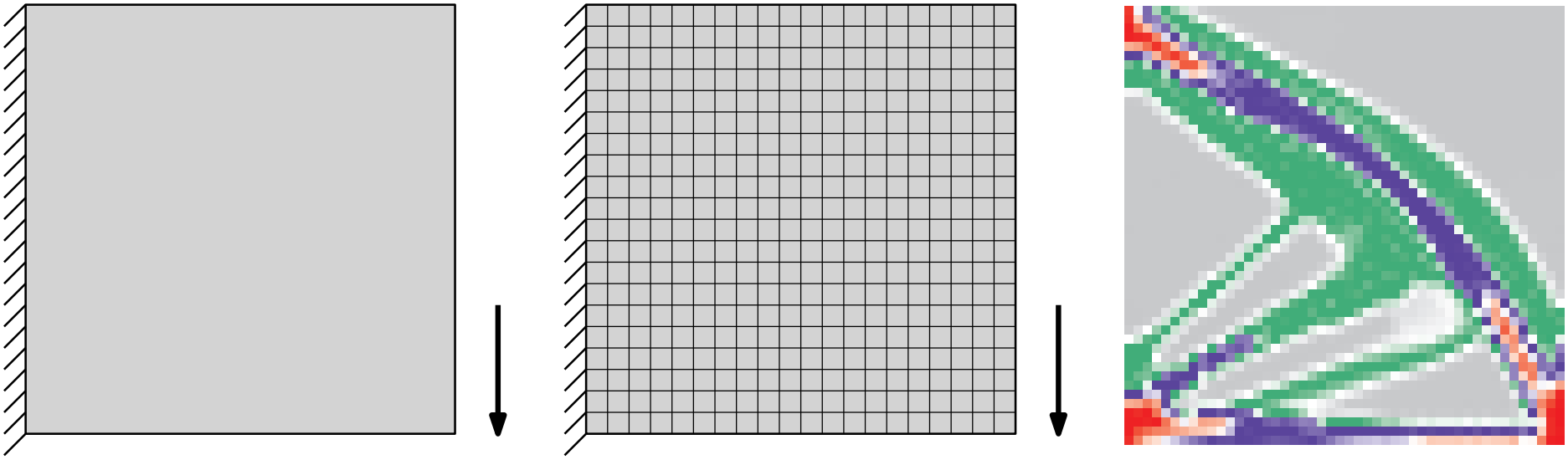
Polymer-based multimaterial



Chris Williams, Virginia Tech

Topology optimization: The essential ideas



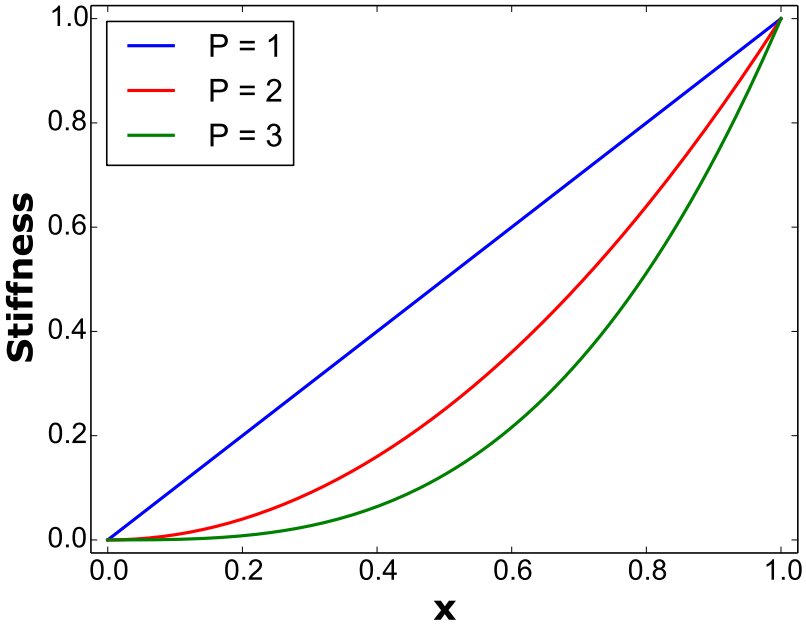
Problem domain

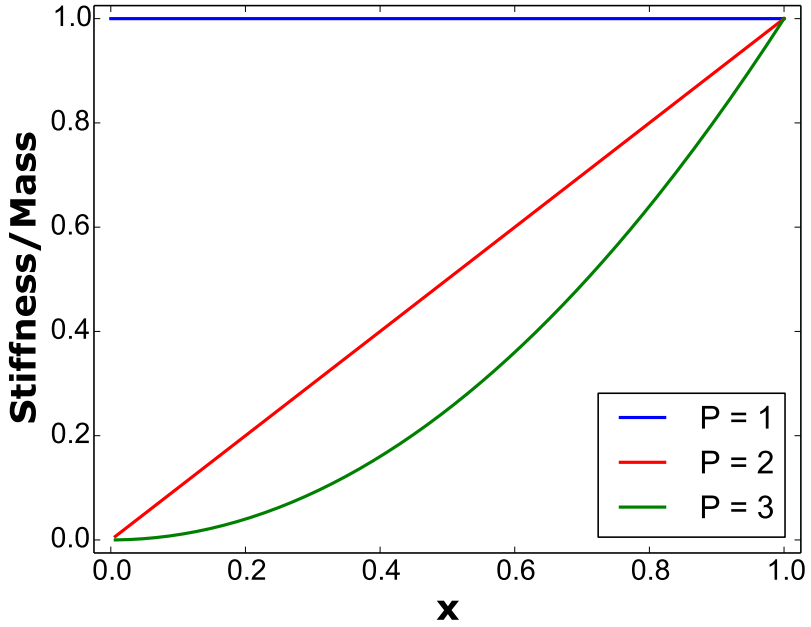
Discretization

Optimize

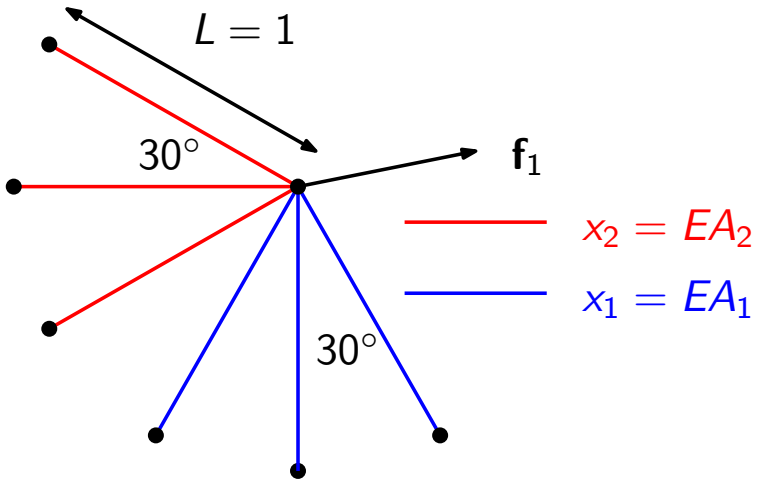
Penalization: Achieving a nearly discrete design

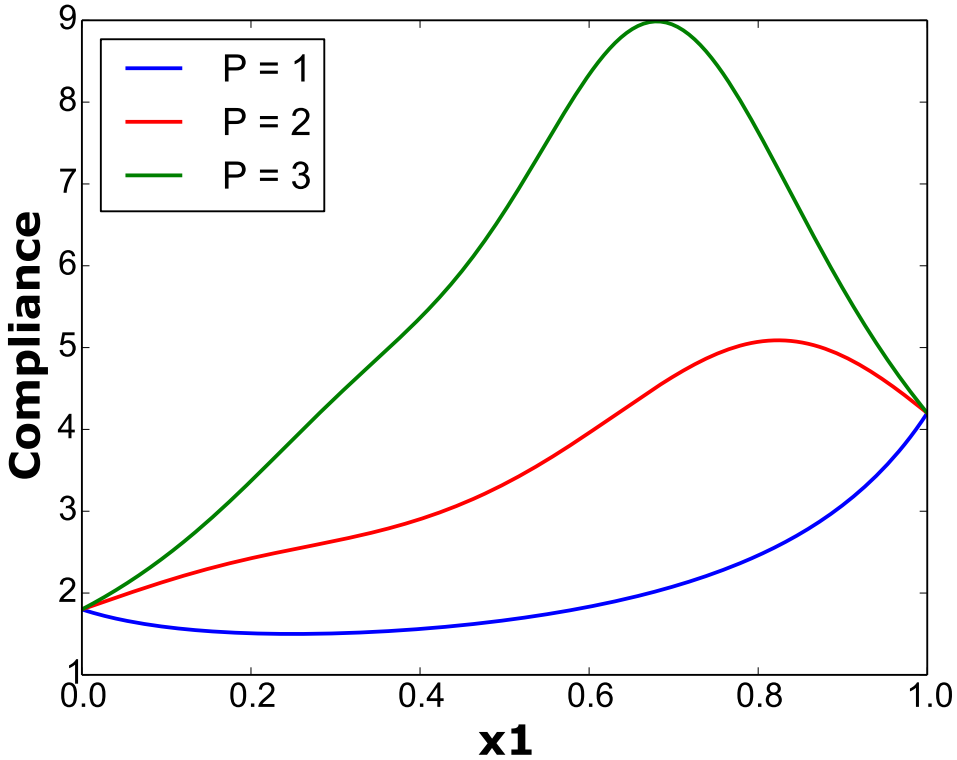
$$E = x^P E_0 \qquad \rho = x\rho_0 \qquad x \in [0, 1]$$





Example: Stolpe–Svanberg truss





- Mass-constrained compliance minimization

$$\begin{aligned} \min_{\mathbf{x}} \quad & \frac{1}{2}\mathbf{f}^T\mathbf{K}(\mathbf{x})^{-1}\mathbf{f} \\ \text{such that} \quad & m(\mathbf{x}) \leq m_{\text{fixed}} \end{aligned}$$

- No adjoint required: $\psi = \mathbf{u}$

$$\frac{df}{dx_i} = -\mathbf{u}^T\frac{\partial \mathbf{K}}{\partial x_i}\mathbf{u}$$

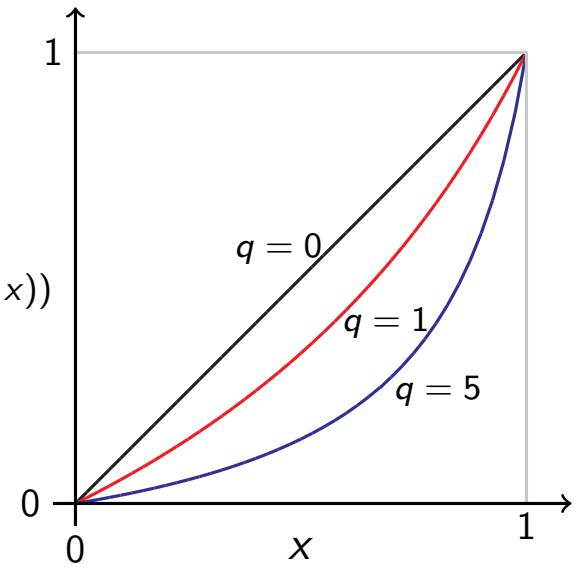
Discrete material optimization (DMO)

- Combined discrete material and topology optimization problem proposed by Sørensen and Lund [8]
- $\mathbf{x} \in \mathbb{R}^{N+1}$: 1 topology variable, N material selection variables
- RAMP-based penalization scheme for stiffness/density interpolation:

$$\mathbf{C}(\mathbf{x}) = \underbrace{\frac{x_1}{1+q(1-x_1)}}_{\text{topology}} \underbrace{\left[\sum_{j=1}^{N} \frac{x_{j+1}}{1+q(1-x_{j+1})} \mathbf{C}_j\right]}_{\text{material selection}}$$

$$\rho(\mathbf{x}) = x_1 \sum_{j=1}^{N} x_{j+1}\rho_j$$

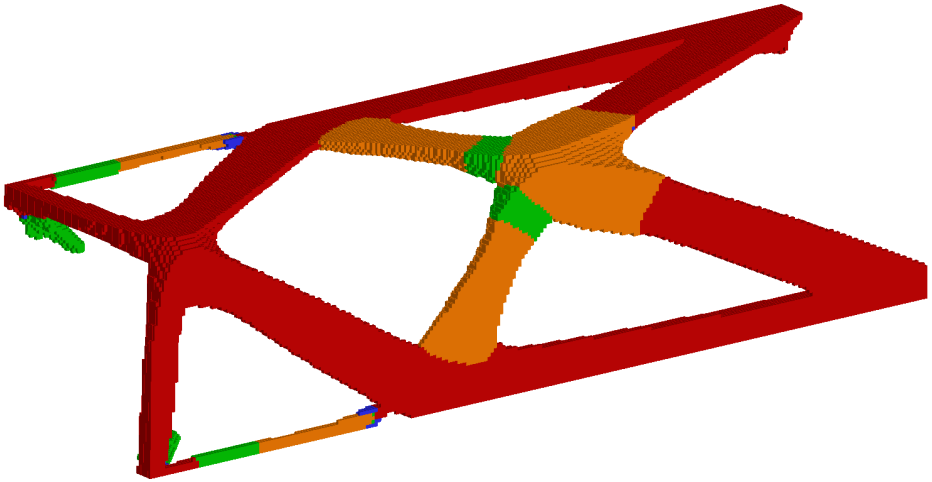
RAMP penalty: $x/(1+q(1-x))$

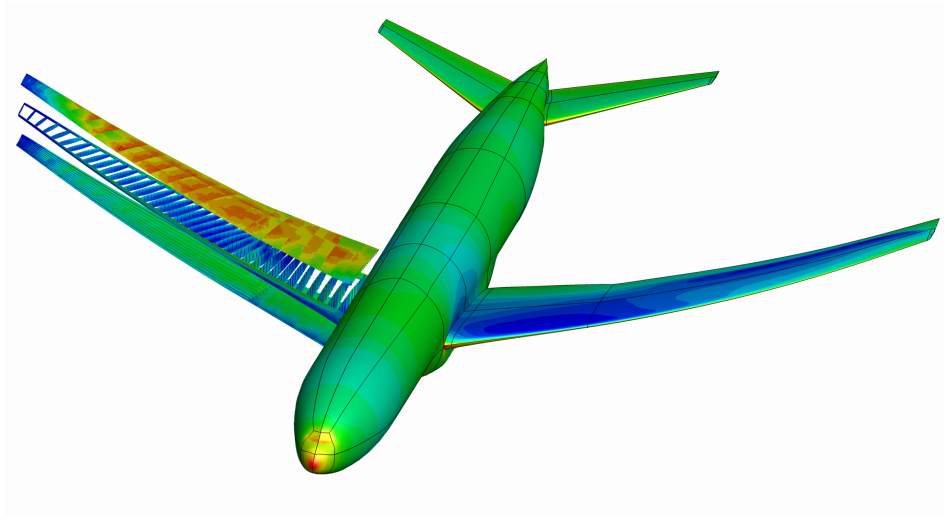


- One catch: Partition of unity constraint for each group of variables:

$$\sum_{j=1}^{N} x_{j+1} = 1$$

The need for large-scale topology optimization





Kenway, Kennedy, Martins [7]

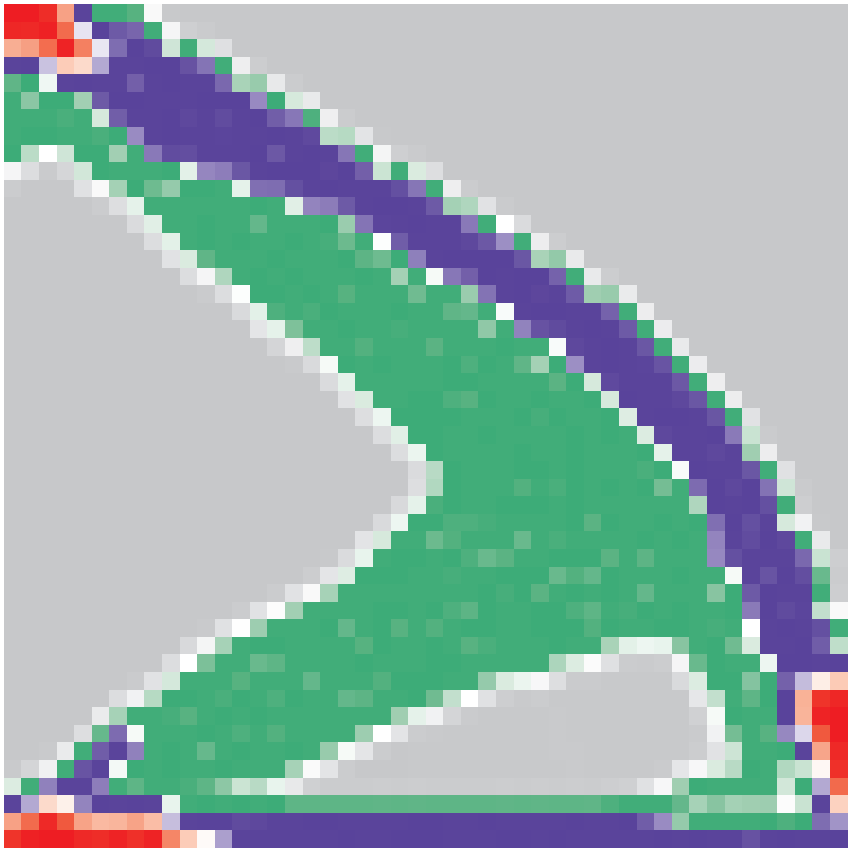
- Aerospace structures are high-aspect ratio/low volume fraction
- Very large analysis and design optimization problems

  Example: Common Research Model

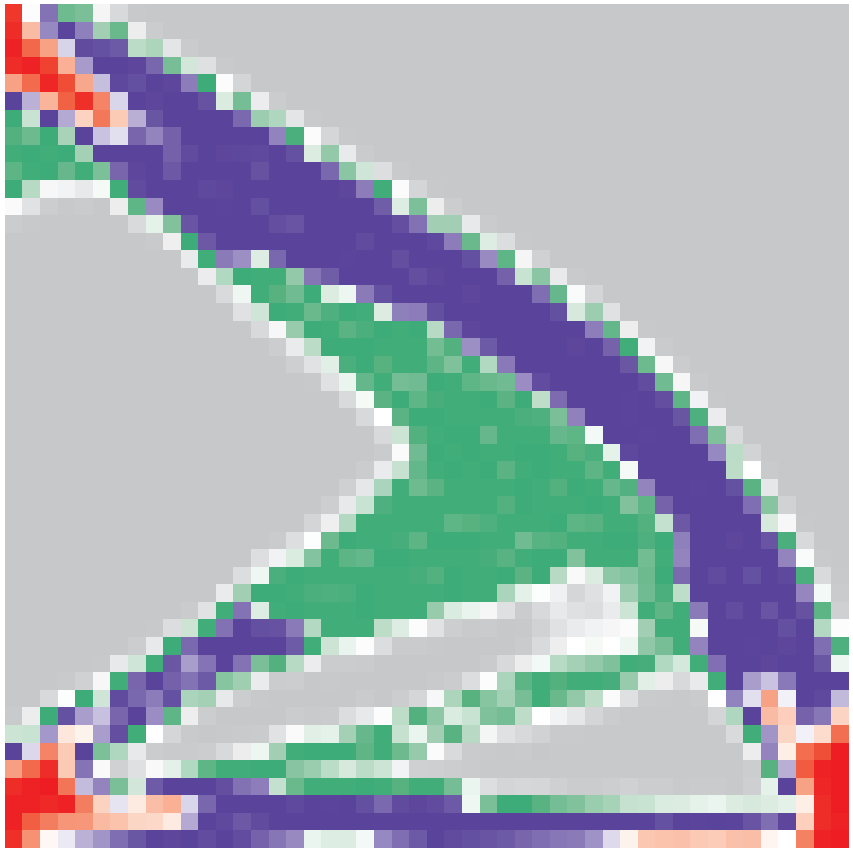
  - $n_{\text{depth}} = 32$ elements through-thickness
  - $(t/c)_{\text{average}} = 0.14$ and $AR = 9$
  - Number of elements $\approx$ 15 million

Compliance minimization vs. stress-based design

Compliance min:



Stress-constrained:



- Compliance minimization and stress-constrained mass minimization lead to different shapes and topologies (Kennedy [3])
- Compliance minimization followed by fixed-topology stress-based shape design leads to different answers

Tailoring optimization algorithms for compliance vs. stress

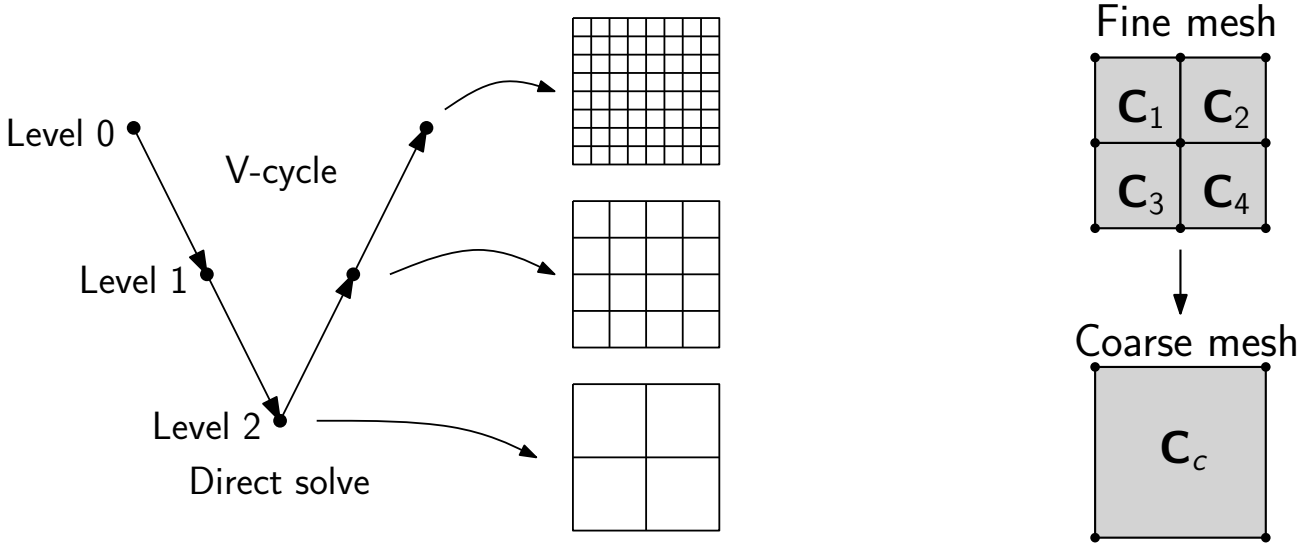
- Compliance and stress-constrained problems have different mathematical properties
- *Different optimization methods required*

Key elements:

- Multigrid preconditioning: scales well with problem size
- Scalable optimization algorithm: Optimization algorithm distributed and parallel
- Scalable gradient evaluation: gradient computation cannot be a bottleneck

A geometric multigrid preconditioner

- Difficulty in topology problems: large changes in stiffness between adjacent regions: $\mathcal{O}(10^6)$ difference
- We evaluate the stiffness on the coarse mesh by computing an average stiffness over the fine mesh:

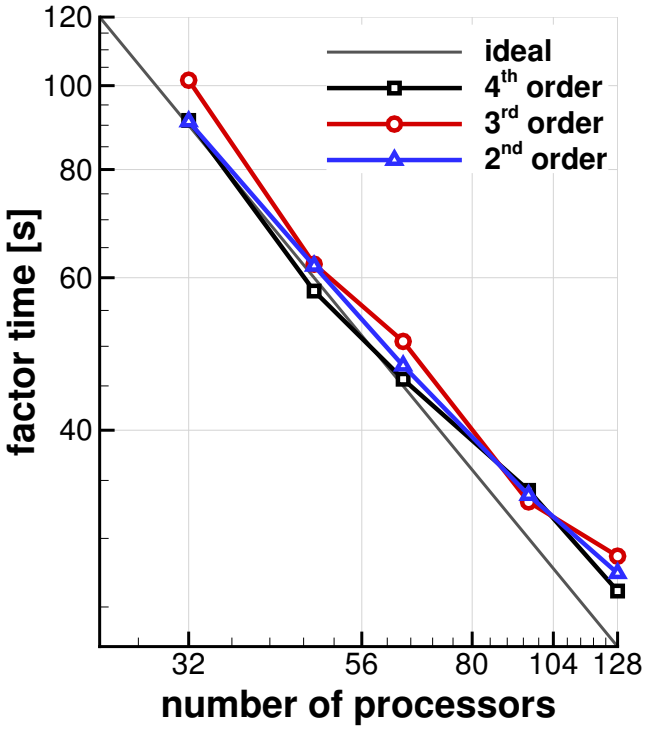


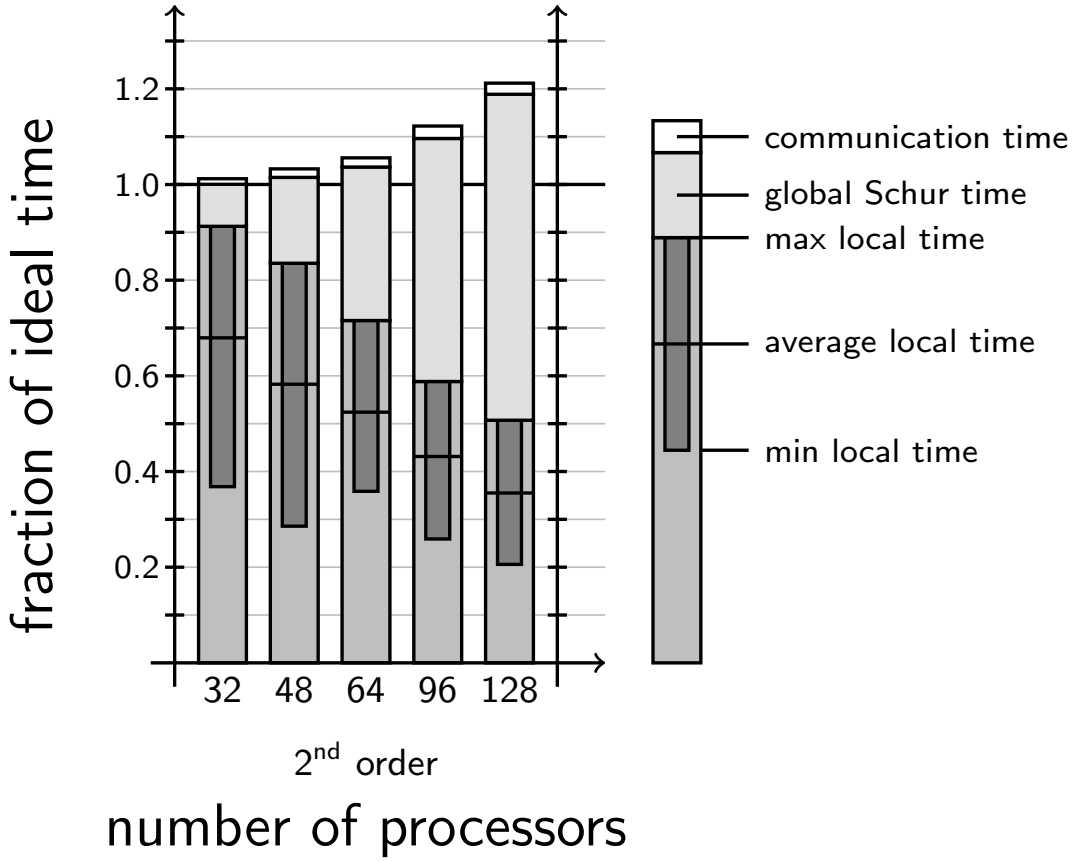
$$\mathbf{C}_c(\mathbf{x}) = \frac{1}{V_f}\int_{V_f} \mathbf{C}(\mathbf{x})\,\mathrm{d}V = \frac{1}{V_f}\sum_i V_i \mathbf{C}_i(\mathbf{x})$$

- We combine multigrid with flexible GMRES to solve the governing equations
- Relatively robust: Solution time roughly doubles between initial (well-scaled) and final (poorly-scaled) designs

Scalable direct solve on the coarse mesh

- Key to robustness: Direct solve on the coarsest mesh
- Schur-complement based factorization scales well with number of processors, but poorly with number of degrees of freedom
  - But the size of the coarse mesh is much smaller





Fast, scalable gradient evaluation

- Gradient evaluation can be a bottleneck [6, 9]
- Special care is required for multimaterial problems with large numbers of design variables per element
  - 4 material problem with 33 filter variables: 165 variables per element
- For compliance, element-by-element gradient evaluation:

$$\nabla_{\mathbf{x}} f = -\underbrace{\sum_e \mathbf{u}_e^T \frac{\partial \mathbf{K}_e}{\partial \mathbf{x}} \mathbf{u}_e}_{\text{sum over elements}} = -\sum_e \underbrace{\sum_q \left[\mathbf{B}_e \mathbf{u}_e\right]^T \frac{\partial \mathbf{C}}{\partial \mathbf{x}} \left[\mathbf{B}_e \mathbf{u}_e\right]}_{\text{sum over quadrature points}}$$

- Generic implementation: Compute the inner product with $\boldsymbol{\psi}$ and $\boldsymbol{\phi}$:

$$\mathbf{d} \leftarrow \mathbf{d} + \alpha \boldsymbol{\psi}^T \frac{\partial \mathbf{C}}{\partial \mathbf{x}} \boldsymbol{\phi}$$

- Best performance for few functions of interest, many design variables per element

Parallel interior-point method for large-scale design

- Optimization cost is small for moderate-scale problems; much more significant for large-scale problems
- To achieve good parallel scalability for large-scale design problems, we implement parallel optimization methods
- Interior-point methods: More complex parallel implementation compared to the method of moving asymptotes (MMA), but better for MDO applications
- Algorithm details:
  - Limited-memory BFGS update scheme for the approximate Hessian of the Lagrangian with damped updates
  - Line-search interior-point method with standard techniques for the Fiacco–McCormick barrier update

Optimization problem structure

- Our interior-point method is based on the following problem structure:

$$\begin{aligned} \text{minimize} \quad & f(\mathbf{x}, \mathbf{u}(\mathbf{x})) \\ \text{with respect to} \quad & \mathbf{x} \\ \text{such that} \quad & \mathbf{x}_l \leq \mathbf{x} \leq \mathbf{x}_u \\ & \mathbf{c}(\mathbf{x}, \mathbf{u}(\mathbf{x})) \geq 0 \\ & \mathbf{c}_s(\mathbf{x}) \geq 0 \\ \text{governed by} \quad & \mathbf{K}(\mathbf{x})\mathbf{u} = \mathbf{f} \end{aligned}$$

- The constraints are divided into two sets:
  - *Dense* constraints: $\mathbf{c}(\mathbf{x}, \mathbf{u}(\mathbf{x}))$; $\mathbf{A} = \nabla_{\mathbf{x}}\mathbf{c}(\mathbf{x})$ fully populated
  - *Sparse* constraints $\mathbf{c}_s(\mathbf{x})$; $\mathbf{A}_s = \nabla_{\mathbf{x}}\mathbf{c}_s(\mathbf{x})$ is sparse
- Dense constraints store on all procs; sparse constraints distributed
- $\mathbf{A}_s$ has a special structure such the product is block diagonal for any diagonal matrix $\mathbf{D}$:

$$\mathbf{A}_s\mathbf{D}\mathbf{A}_s^T = \mathbf{G} = \text{diag}\{\mathbf{G}_{11}, \mathbf{G}_{22}, \ldots, \mathbf{G}_{qq}\}$$

- DMO constraints fit this structure

Implementing the approximate Newton step in parallel

- At each step in the interior-point method, we compute a search direction by solving the linearized optimality conditions
- After manipulation, this system takes the following form:

$$\begin{bmatrix} \mathbf{F} & \mathbf{E}^T \\ \mathbf{E} & \mathbf{A}_s\mathbf{D}^{-1}\mathbf{A}_s^T + \mathbf{G} \end{bmatrix} \begin{bmatrix} \mathbf{p}_z \\ \mathbf{p}_s \end{bmatrix} = \begin{bmatrix} \mathbf{r}_c \\ \mathbf{r}_s \end{bmatrix}$$

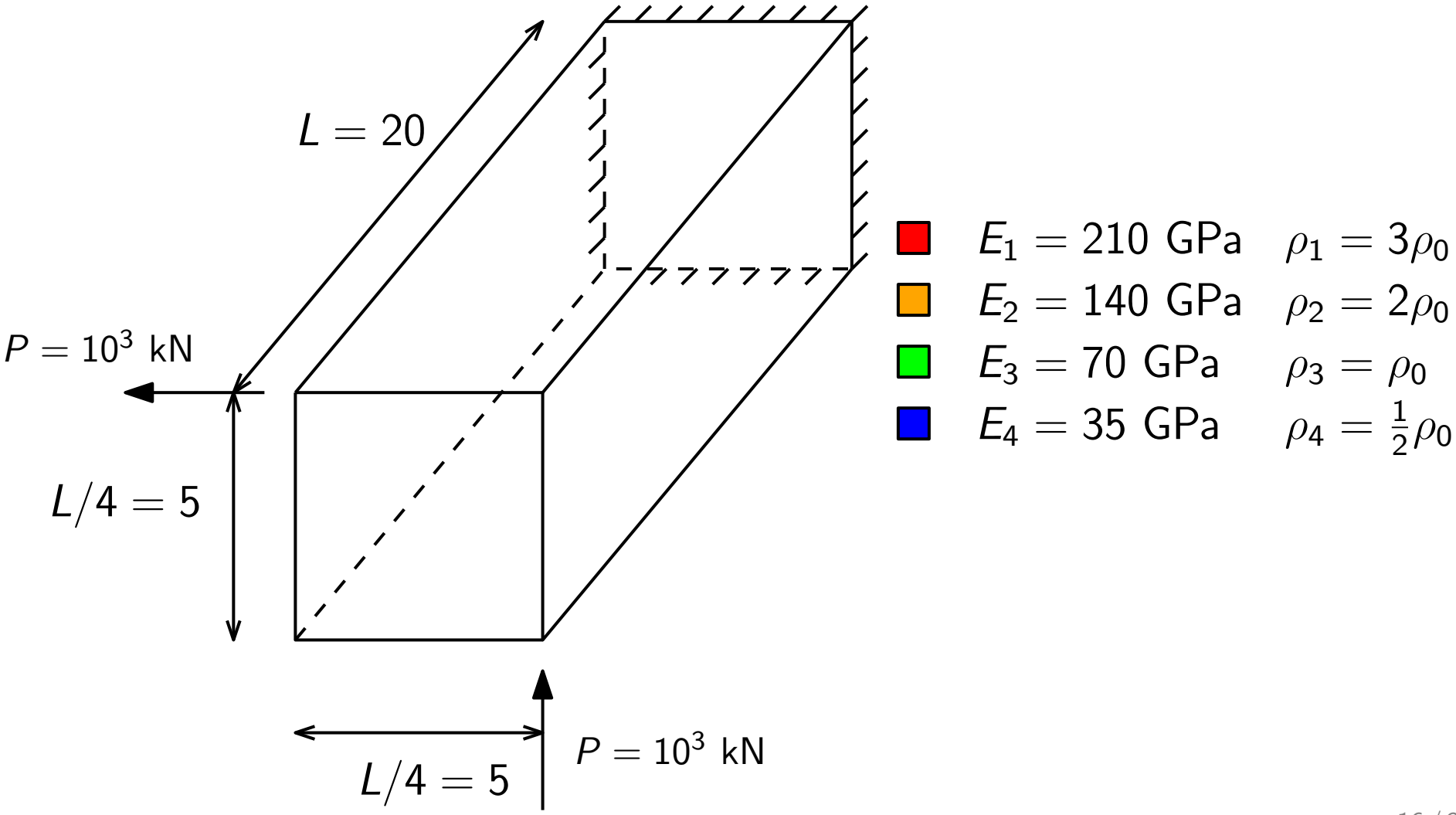
- $\mathbf{F}$ is small, dense, and stored on all procs
- $\mathbf{E}$ is stored as a series of distributed vectors
- The lower block-diagonal $\mathbf{A}_s\mathbf{D}^{-1}\mathbf{A}_s^T + \mathbf{G}$ can be very large, but is distributed and block-diagonal
- We can compute an update using a Schur-complement method - more details in the paper

$$\left[\mathbf{F} - \mathbf{E}^T\left(\mathbf{A}_s\mathbf{D}^{-1}\mathbf{A}_s^T + \mathbf{G}\right)^{-1}\mathbf{E}\right]\mathbf{p}_z = \mathbf{r}$$

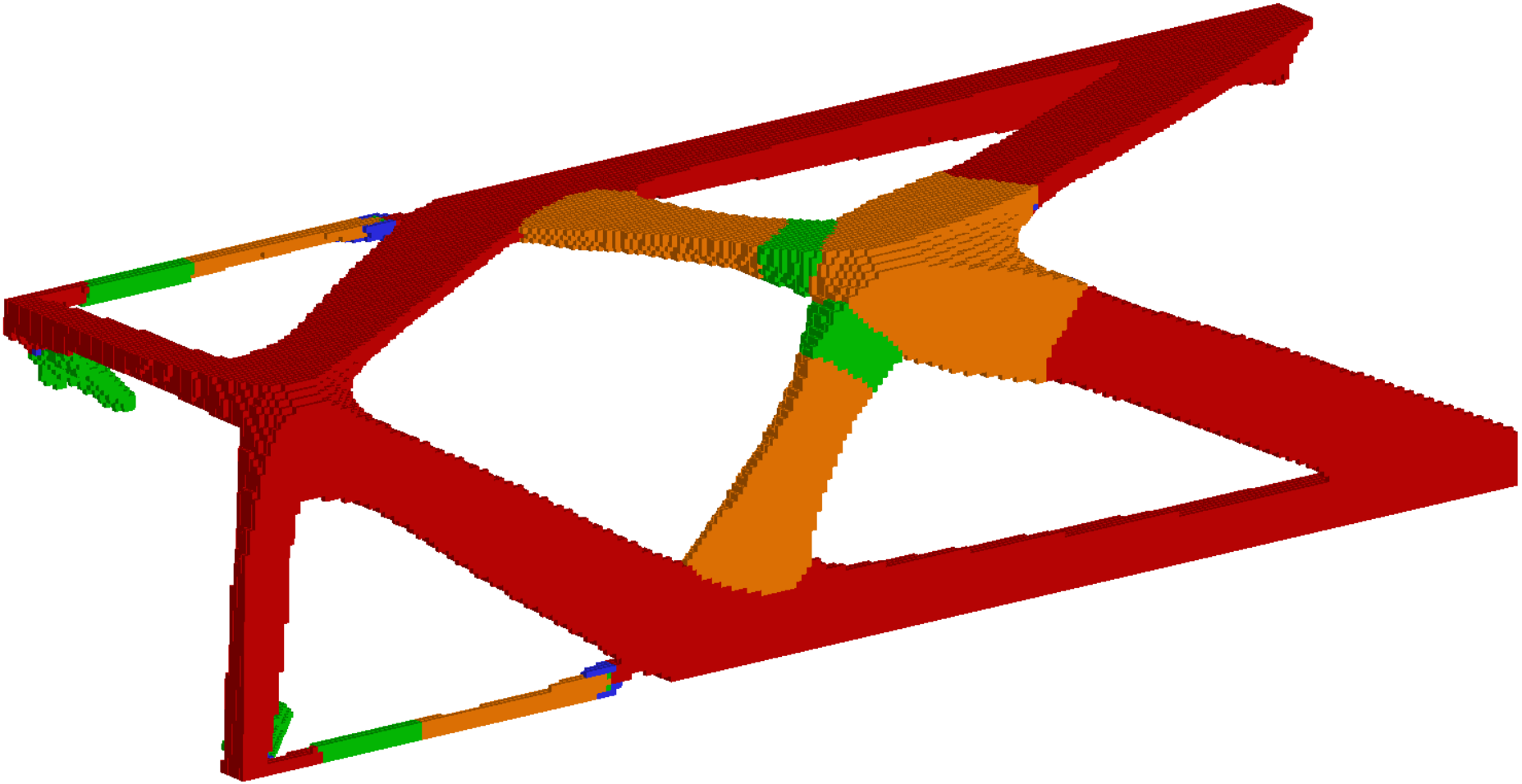
- Sparse constraint structure enables efficient parallel solution

Compliance minimization problem

- Problem discretization: $64 \times 64 \times 256$ elements
- DMO parametrization
- 5.24 million design variables, 1.05 million constraints

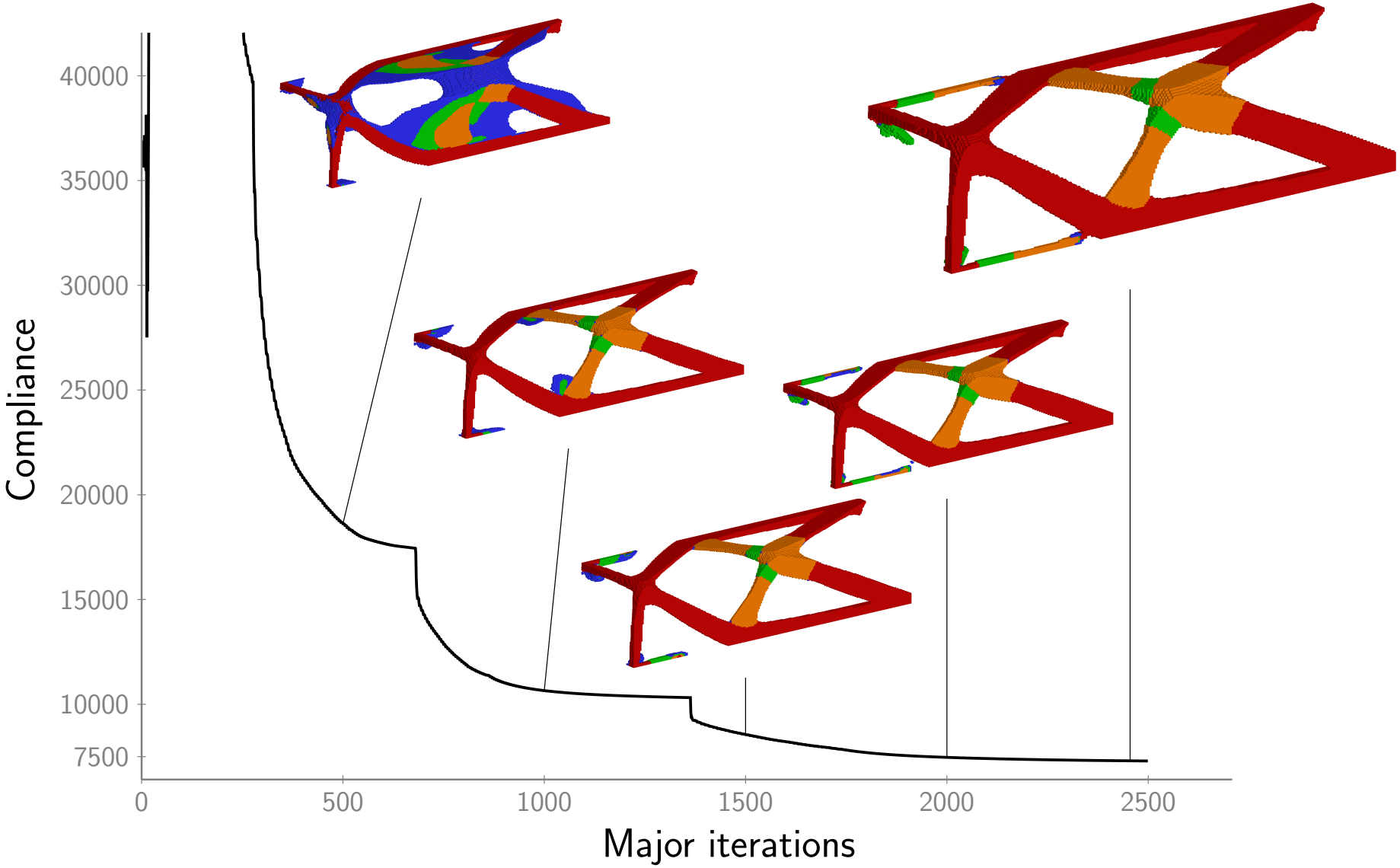


Topology and multimaterial results



- Optimization required 9 hours and 52 minutes of wall time on 32 processors
- 4.2 iterations a minute, or roughly an iteration every 15 seconds

Multimaterial compliance minimization

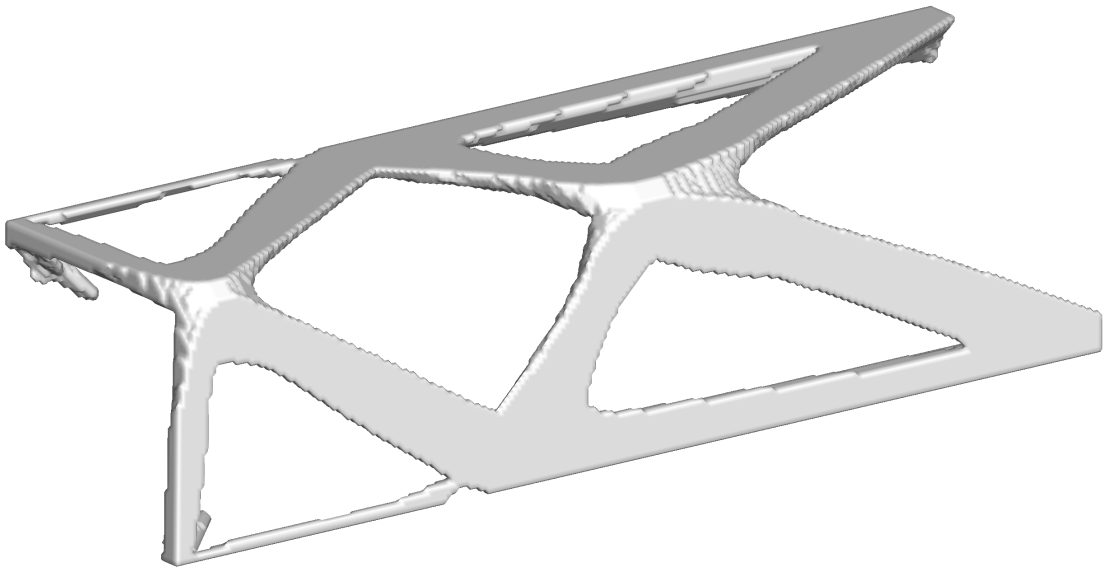


Post-processing and build

- Generated an .stl file from the 0.5-level set of the function:

$$x_1 \max_{j=1,\ldots,N} x_{j+1}$$

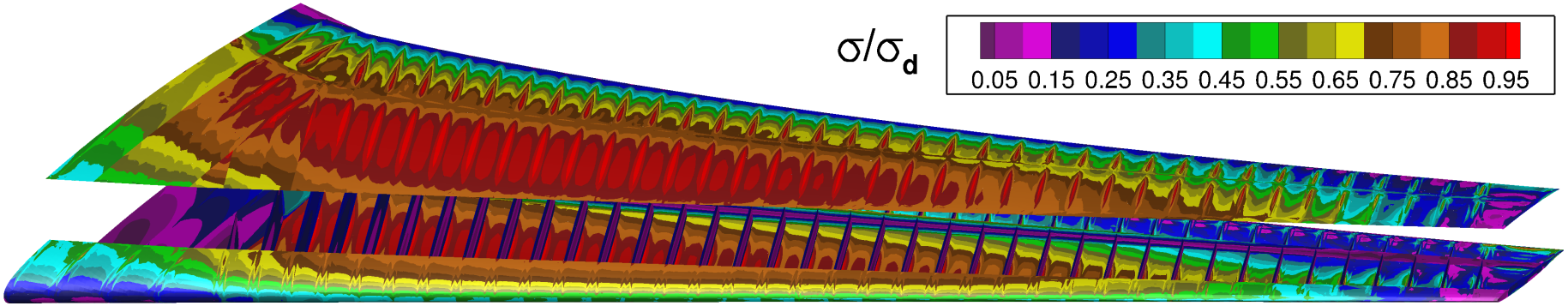
- No post-smoothing applied



- Thanks to Justin Gray (NASA) for printing the structure

Stress-constrained design optimization

- Minimize the structural mass
- Bound a stress measure $\sigma(\xi) \leq \sigma_y$ everywhere within the domain, $\xi \in \Omega$



- $\sigma(\xi) \leq \sigma_y$ is an infinite-dimensional constraint; it must be imposed everywhere in Ω
- We cheat: Impose it at lots of points

Problem formulation: Thickness parametrization

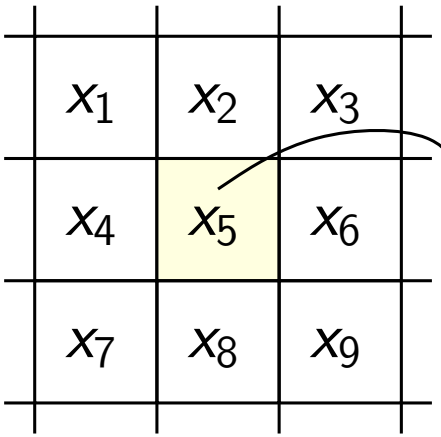
- Start with continuous thickness problems, topology later
- Direct or inverse parametrization for the structural thicknesses

Direct: $t_i = x_i$ Inverse: $t_i = \dfrac{1}{x_i}$

- Mass and stiffness are linear functions of the thickness

$$m(\mathbf{x}) = \mathbf{t}^T \mathbf{m}$$
$$\mathbf{K}(\mathbf{x}) = \sum_i t_i \mathbf{K}_i$$

- Use of a thickness-filter does not alter these expressions



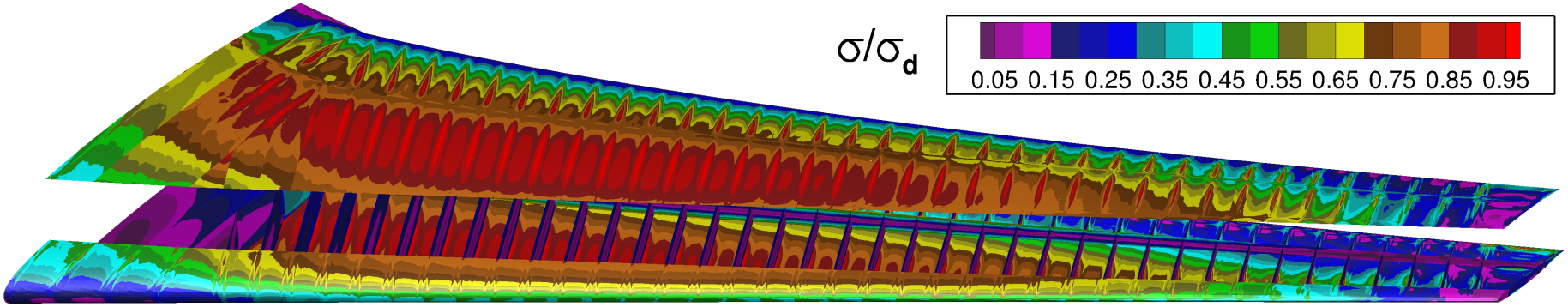
$$t_5 = \sum_{i=1}^{9} w_i x_i$$

Problem formulation: Stress constraint formulations

- We study stress constraints that take the form:

$$g(\xi, \mathbf{u}) = 1 - \mathbf{s}^T\mathbf{h} - \mathbf{s}^T\mathbf{G}\mathbf{s} \geq 0$$

- Scaled stress, $\mathbf{s}(\xi)$, evaluated at a point in the structure $\xi \in \Omega$
- $\mathbf{s}(\xi) = \mathbf{DBu}$ depends on $\mathbf{u}$ but not $\mathbf{x}$ directly



- Many failure criteria take this form, e.g.

Von Mises:

$$\mathbf{s} = \frac{1}{\sigma_s}\begin{bmatrix}\sigma_x \\ \sigma_y \\ \sigma_{xy}\end{bmatrix} \qquad \mathbf{G} = \begin{bmatrix} 1 & -\frac{1}{2} & \\ -\frac{1}{2} & 1 & \\ & & 3 \end{bmatrix} \quad \mathbf{h} = \begin{bmatrix}0\\0\\0\end{bmatrix}$$

- Note: $\mathbf{G}$ is positive definite, so $g(\xi, \mathbf{u})$ is concave!

Optimization using reduced-space methods

Full-space problem:

$$\begin{aligned} \text{minimize} \quad & m(\mathbf{x}) \\ \text{with respect to} \quad & \mathbf{x} \geq 0,\ \mathbf{u} \\ \text{such that} \quad & g(\xi_i, \mathbf{u}) \geq 0 \\ & \mathbf{K}(\mathbf{x})\mathbf{u} = \mathbf{f} \end{aligned}$$

- If direct parametrization used, non-convexity only enters through the governing equation

Optimization using reduced-space methods

Reduced-space problem:

$$\begin{aligned} \text{minimize} \quad & m(\mathbf{x}) \\ \text{with respect to} \quad & \mathbf{x} \geq 0 \\ \text{such that} \quad & g(\xi_i, \mathbf{u}(\mathbf{x})) \geq 0 \\ \text{governed by} \quad & \mathbf{K}(\mathbf{x})\mathbf{u} = \mathbf{f} \end{aligned}$$

- Convexity properties destroyed due to $\mathbf{u}(\mathbf{x})$

Optimization using reduced-space methods

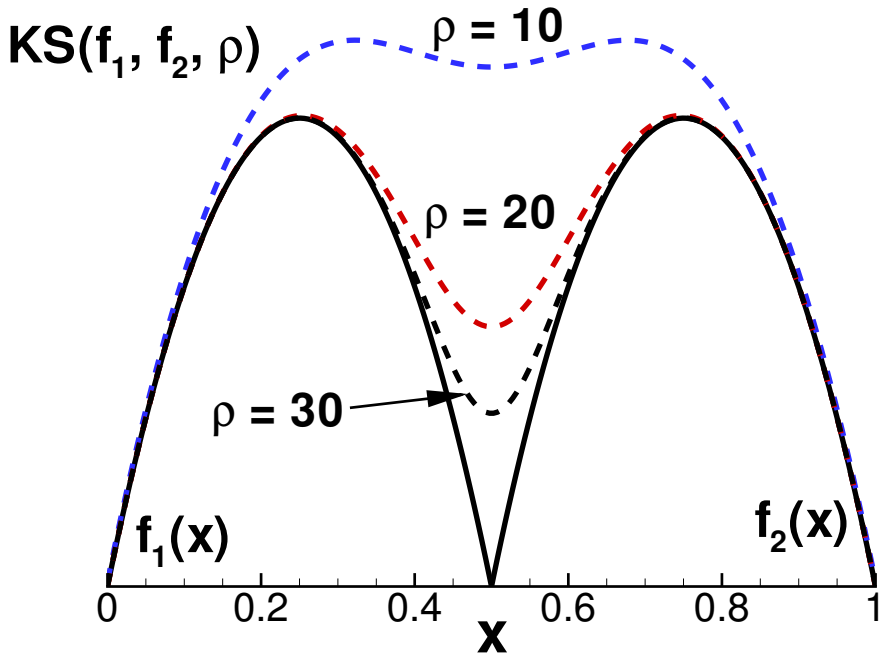
Aggregation-constrained reduced space problem:

$$\begin{aligned} \text{minimize} \quad & m(\mathbf{x}) \\ \text{with respect to} \quad & \mathbf{x} \geq 0 \\ \text{such that} \quad & c(g(\xi_i, \mathbf{u}), \rho) \geq 0 \\ \text{governed by} \quad & \mathbf{K}(\mathbf{x})\mathbf{u} = \mathbf{f} \end{aligned}$$

Aggregation functionals:

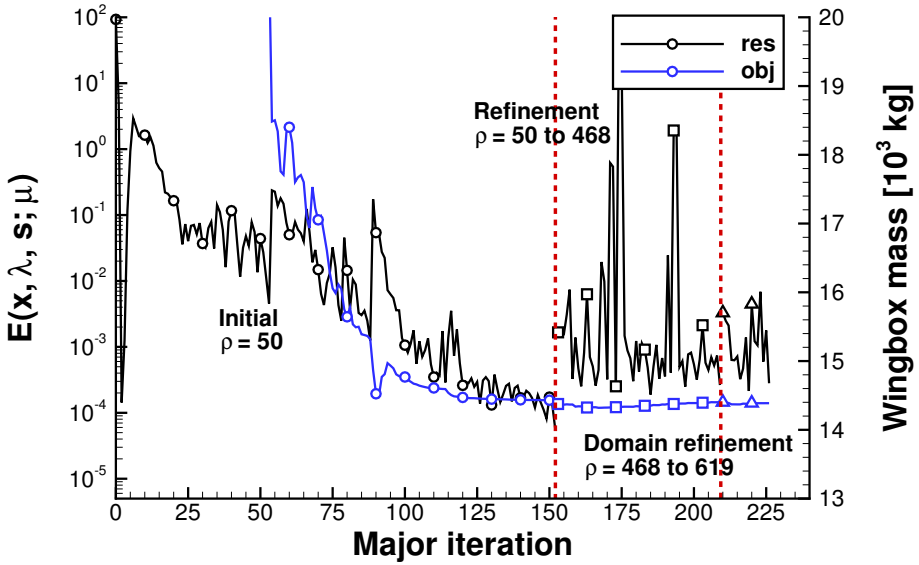
$$c_{\mathrm{KS}}(g, \rho) = -\frac{1}{\rho} \ln \left[\sum e^{-\rho g_i} \right]$$

$$c_{\mathrm{IE}}(g, \rho) = \frac{\sum g e^{-\rho g}}{\sum e^{-\rho g}}$$

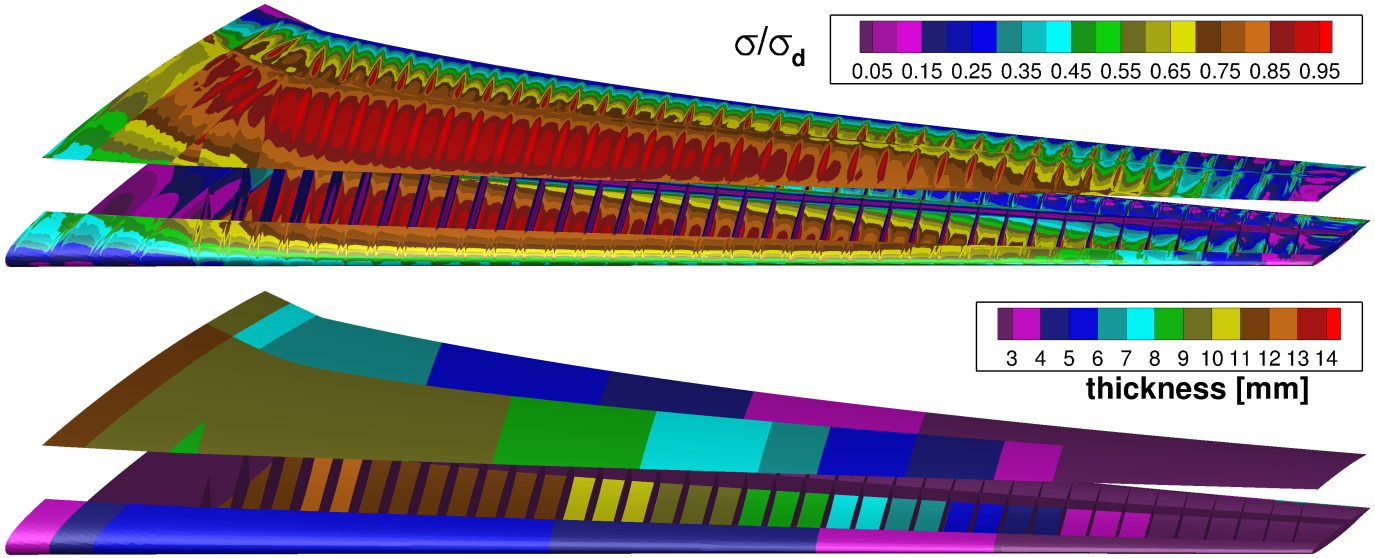


Issues with constraint aggregation

- Aggregation constraints are very nonlinear
- Adaptive aggregation methods can be used, but pose issues for very large design problems



Kennedy and Hicken [6, 5, 4]



Full-space barrier methods

$$\begin{aligned} \text{min} \quad & m(\mathbf{x}) \\ \text{with respect to} \quad & \mathbf{x} \geq 0,\ \mathbf{u} \\ \text{such that} \quad & g(\xi_i, \mathbf{u}) \geq 0 \quad \mathbf{K}(\mathbf{x})\mathbf{u} = \mathbf{f} \end{aligned}$$

- Impose the governing equation as an equality constraint
- Move the stress-constraints into the object through a barrier term

$$\begin{aligned} \min_{\mathbf{x},\mathbf{u}} \quad & m(\mathbf{x}) - \mu \sum_{i=1}^{n} \ln x_i - \mu \sum_{i=1}^{N} \ln g(\xi_i, \mathbf{u}) \\ \text{such that} \quad & \mathbf{K}(\mathbf{x})\mathbf{u} = \mathbf{f} \end{aligned}$$

- Minimize for a sequence of decreasing μ
- Issue: Problem becomes poorly scaled for small μ

Full-space barrier methods

- The Lagrangian for the problem is:

$$\mathcal{L}(\mathbf{x}, \mathbf{u}, \boldsymbol{\psi}) = m(\mathbf{x}) - \mu \sum_{i=1}^{n} \ln x_i - \mu \sum_{i=1}^{N} \ln g(\xi_i, \mathbf{u}) + \boldsymbol{\psi}^T (\mathbf{K}(\mathbf{x})\mathbf{u} - \mathbf{f})$$

- The KKT conditions for the barrier problem take the form:

$$\begin{aligned} \mathbf{r}_x &= \nabla_{\mathbf{x}} m - \mu \mathbf{X}^{-1}\mathbf{e} + \mathbf{A}(\mathbf{x}, \mathbf{u})^T \boldsymbol{\psi} &= 0 \\ \mathbf{r}_u &= \mathbf{K}(\mathbf{x})\boldsymbol{\psi} - \mu \mathbf{g} &= 0 \\ \mathbf{r}_\psi &= \mathbf{K}(\mathbf{x})\mathbf{u} - \mathbf{f} &= 0 \end{aligned}$$

- Derivatives of the governing equation with respect to the design variables:

$$\mathbf{A}(\mathbf{x}, \mathbf{u}) = \frac{\partial \mathbf{K}(\mathbf{x})\mathbf{u}}{\partial \mathbf{x}}$$

- Independent of $\mathbf{x}$ for the direct parametrization

Newton method for the full-space barrier problem

- Solve the Newton system inexactly with FGMRES for the step:

$$\begin{bmatrix} \nabla_{\mathbf{xx}}\mathcal{L} & \mathbf{A}(\mathbf{x},\boldsymbol{\psi})^T & \mathbf{A}(\mathbf{x},\mathbf{u})^T \\ \mathbf{A}(\mathbf{x},\boldsymbol{\psi}) & \mu\mathbf{C} & \mathbf{K}(\mathbf{x}) \\ \mathbf{A}(\mathbf{x},\mathbf{u}) & \mathbf{K}(\mathbf{x}) & \end{bmatrix} \begin{bmatrix} \Delta\mathbf{x} \\ \Delta\mathbf{u} \\ \Delta\boldsymbol{\psi} \end{bmatrix} = - \begin{bmatrix} \mathbf{r}_{\mathbf{x}} \\ \mathbf{r}_{\mathbf{u}} \\ \mathbf{r}_{\psi} \end{bmatrix}$$

- Hessian of the Lagrangian takes different forms depending on the parametrization
  - Direct parametrization:

$$\nabla_{\mathbf{xx}}\mathcal{L} = \mu\mathbf{X}^{-2}$$

  - Inverse parametrization:

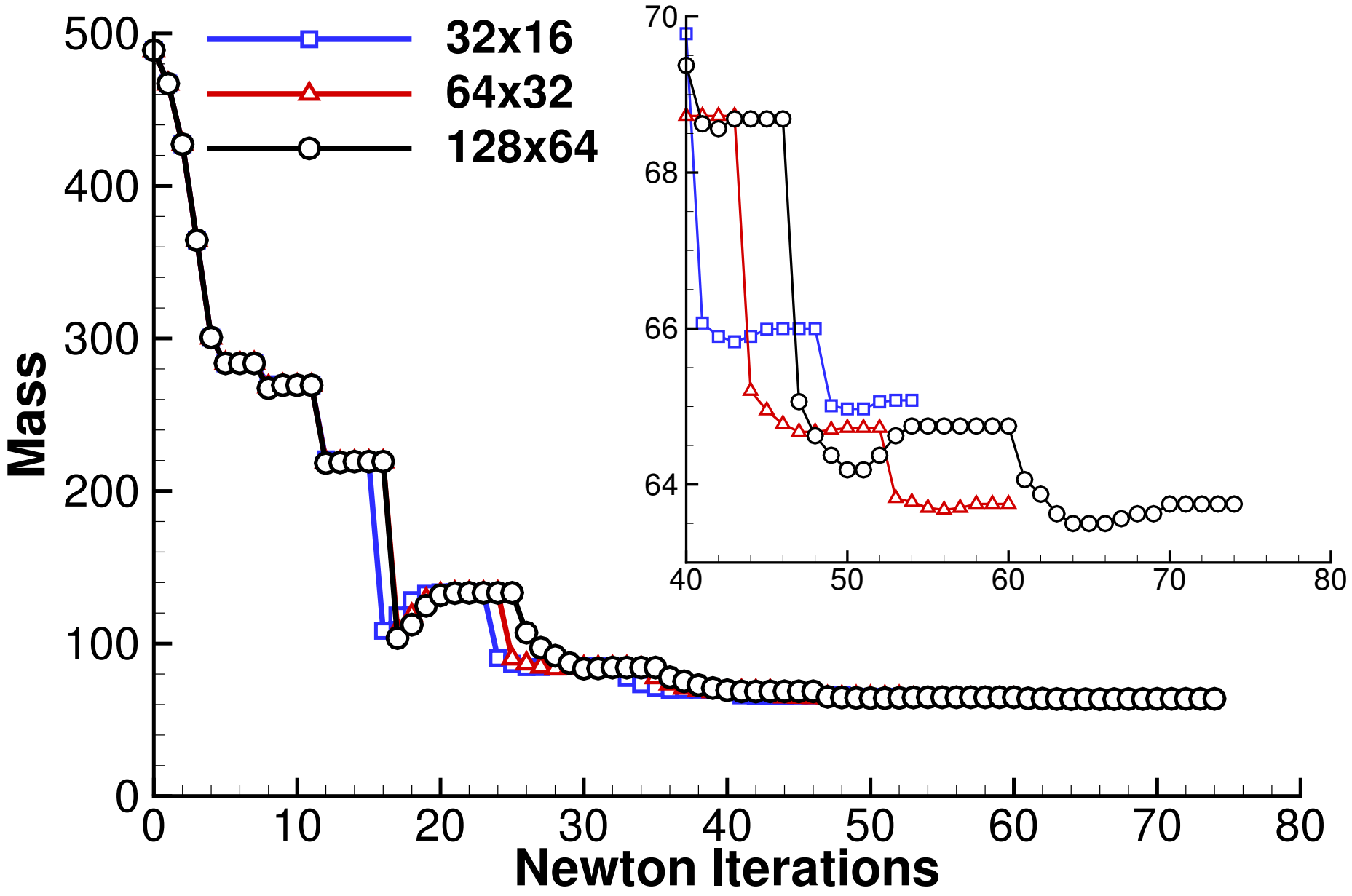
$$\nabla_{\mathbf{xx}}\mathcal{L} = \nabla_{\mathbf{xx}}m + \mu\mathbf{X}^{-2} + \nabla_{\mathbf{xx}}(\boldsymbol{\psi}^T\mathbf{K}(\mathbf{x})\mathbf{u})$$

- $\mathbf{X}^{-2}$ and $\nabla_{\mathbf{xx}}m$ are positive definite
- $\nabla_{\mathbf{xx}}(\boldsymbol{\psi}^T\mathbf{K}(\mathbf{x})\mathbf{u})$ may be indefinite

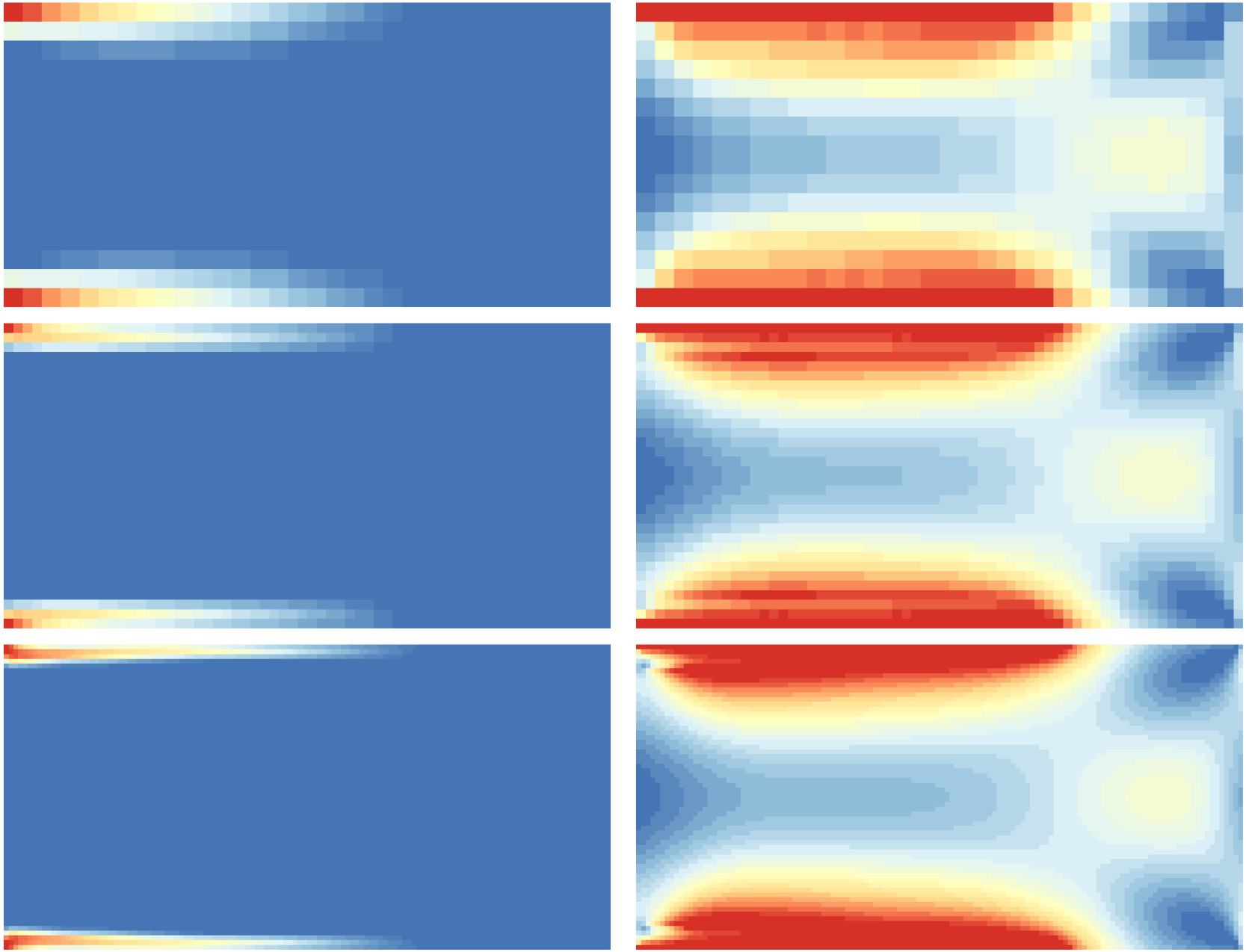
Results for direct thickness parametrization

- Discretization using either 32×16, 64×32, or 128×64 elements/design variables

Mass minimization results



Design and stress



Topology optimization: Unfortunate complications

1. Penalization (e.g. RAMP, SIMP) with $t \in (0, 1]$
   - Penalization only affects the governing equations
2. ϵ-relaxation to avoid stress singularity (Allows large stresses in elements with small thicknesses)
   - ϵ-relaxation requires adding terms to the stress-constraints

$$g(\xi, \mathbf{u}, \mathbf{x}) = 1 + \frac{\epsilon}{t} - \epsilon - \mathbf{s}^T\mathbf{h} - \mathbf{s}^T\mathbf{G}\mathbf{s} \geq 0$$

   - Pick small $\epsilon > 0$, as $t \to 0$, stress constraint is always satisfied
   - Direct parametrization: non-concave

$$g(\xi, \mathbf{u}, \mathbf{x}) = 1 + \frac{\epsilon}{x} - \epsilon - \mathbf{s}^T\mathbf{h} - \mathbf{s}^T\mathbf{G}\mathbf{s} \geq 0$$

   - Inverse parametrization: concave

$$g(\xi, \mathbf{u}, \mathbf{x}) = 1 + \epsilon x - \epsilon - \mathbf{s}^T\mathbf{h} - \mathbf{s}^T\mathbf{G}\mathbf{s} \geq 0$$

Newton system for the topology optimization problem

$$\begin{bmatrix} \nabla_{\mathbf{xx}}\mathcal{L} & \mathbf{A}(\mathbf{x},\boldsymbol{\psi})^T + \mu\mathbf{C}_{\mathbf{ux}}^T & \mathbf{A}(\mathbf{x},\mathbf{u})^T \\ \mathbf{A}(\mathbf{x},\boldsymbol{\psi}) + \mu\mathbf{C}_{\mathbf{ux}} & \mu\mathbf{C} & \mathbf{K}(\mathbf{x}) \\ \mathbf{A}(\mathbf{x},\mathbf{u}) & \mathbf{K}(\mathbf{x}) & \end{bmatrix} \begin{bmatrix} \Delta\mathbf{x} \\ \Delta\mathbf{u} \\ \Delta\boldsymbol{\psi} \end{bmatrix} = - \begin{bmatrix} \mathbf{r}_{\mathbf{x}} \\ \mathbf{r}_{\mathbf{u}} \\ \mathbf{r}_{\psi} \end{bmatrix}$$

- $\mathbf{K}(\mathbf{x})$ is not a linear function of $\mathbf{x}$ due to penalization
  - Direct parametrization:

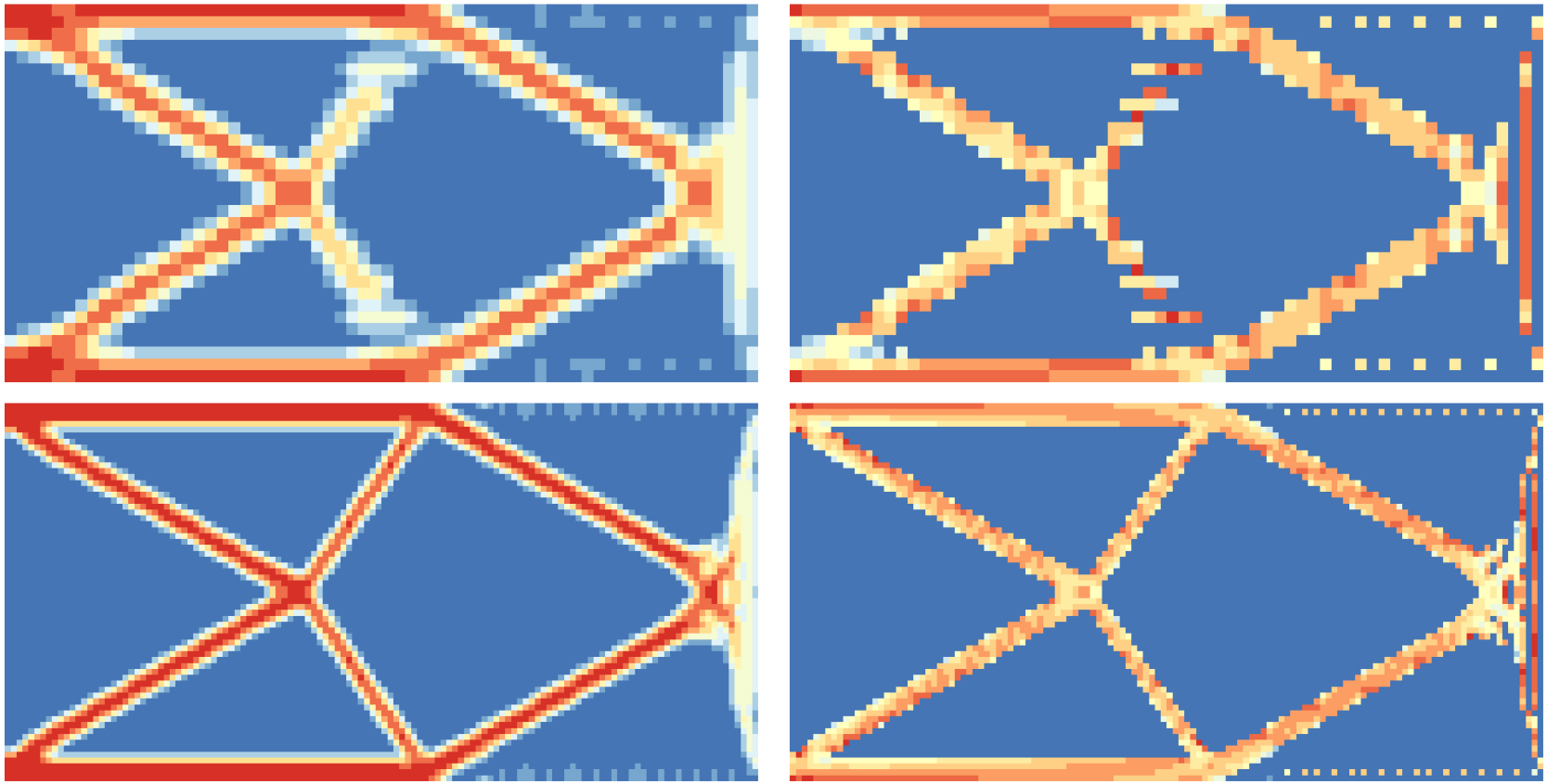
$$\nabla_{\mathbf{xx}}\mathcal{L} = \mu\mathbf{X}^{-2} + \mu\mathbf{C}_{\mathbf{xx}} + \nabla_{\mathbf{xx}}(\boldsymbol{\psi}^T\mathbf{K}(\mathbf{x})\mathbf{u})$$

  - Inverse parametrization:

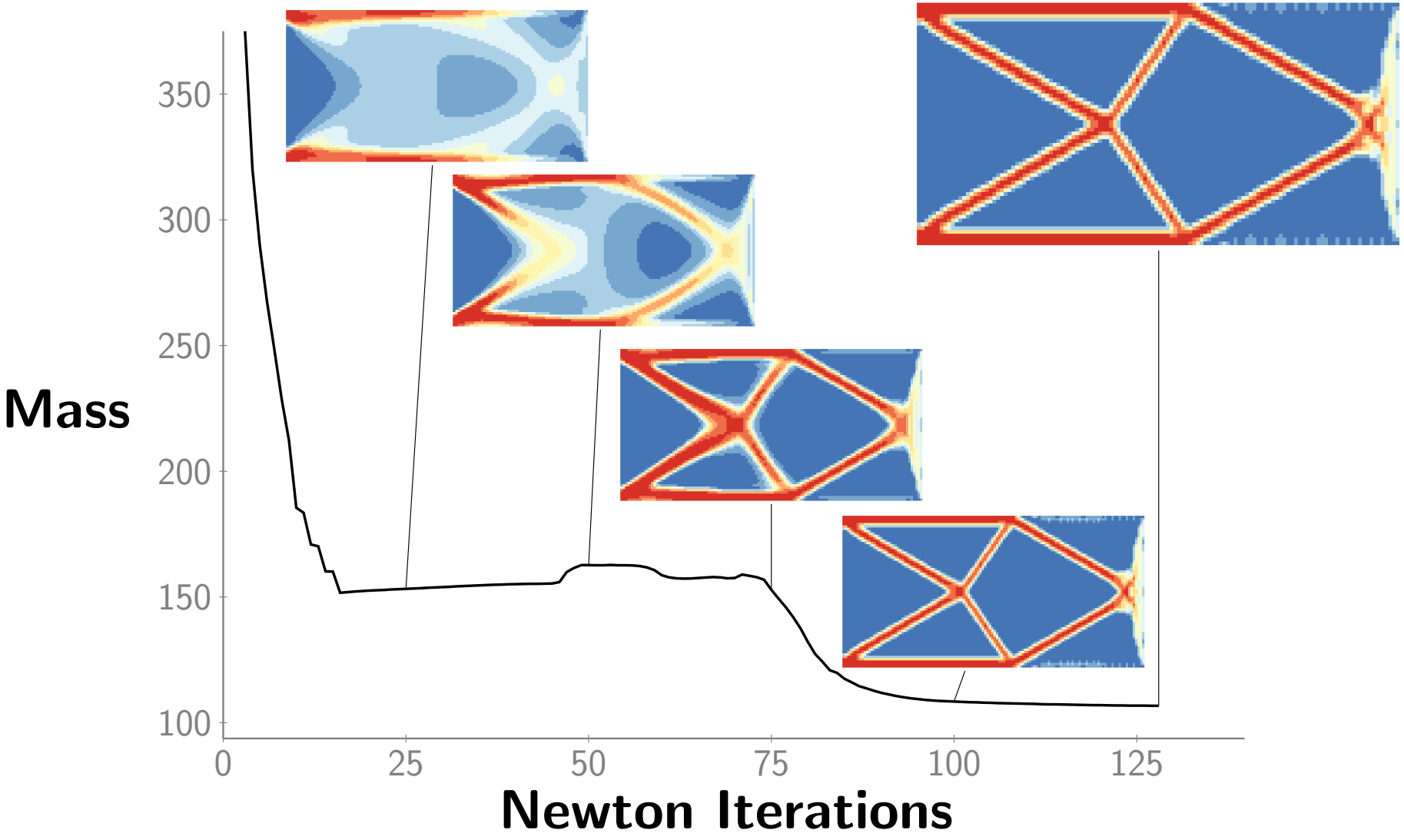
$$\nabla_{\mathbf{xx}}\mathcal{L} = \nabla_{\mathbf{xx}}m + \mu\mathbf{X}^{-2} + \mu\mathbf{C}_{\mathbf{xx}} + \nabla_{\mathbf{xx}}(\boldsymbol{\psi}^T\mathbf{K}(\mathbf{x})\mathbf{u})$$

- Direct parametrization: $\mathbf{C}_{\mathbf{xx}}$ is indefinite since the constraint contains $1/x$ term
- Inverse parametrization: $\mathbf{C}_{\mathbf{xx}}$ is positive definite
  - Use inverse parametrization and discard $\nabla_{\mathbf{xx}}(\boldsymbol{\psi}^T\mathbf{K}(\mathbf{x})\mathbf{u})$

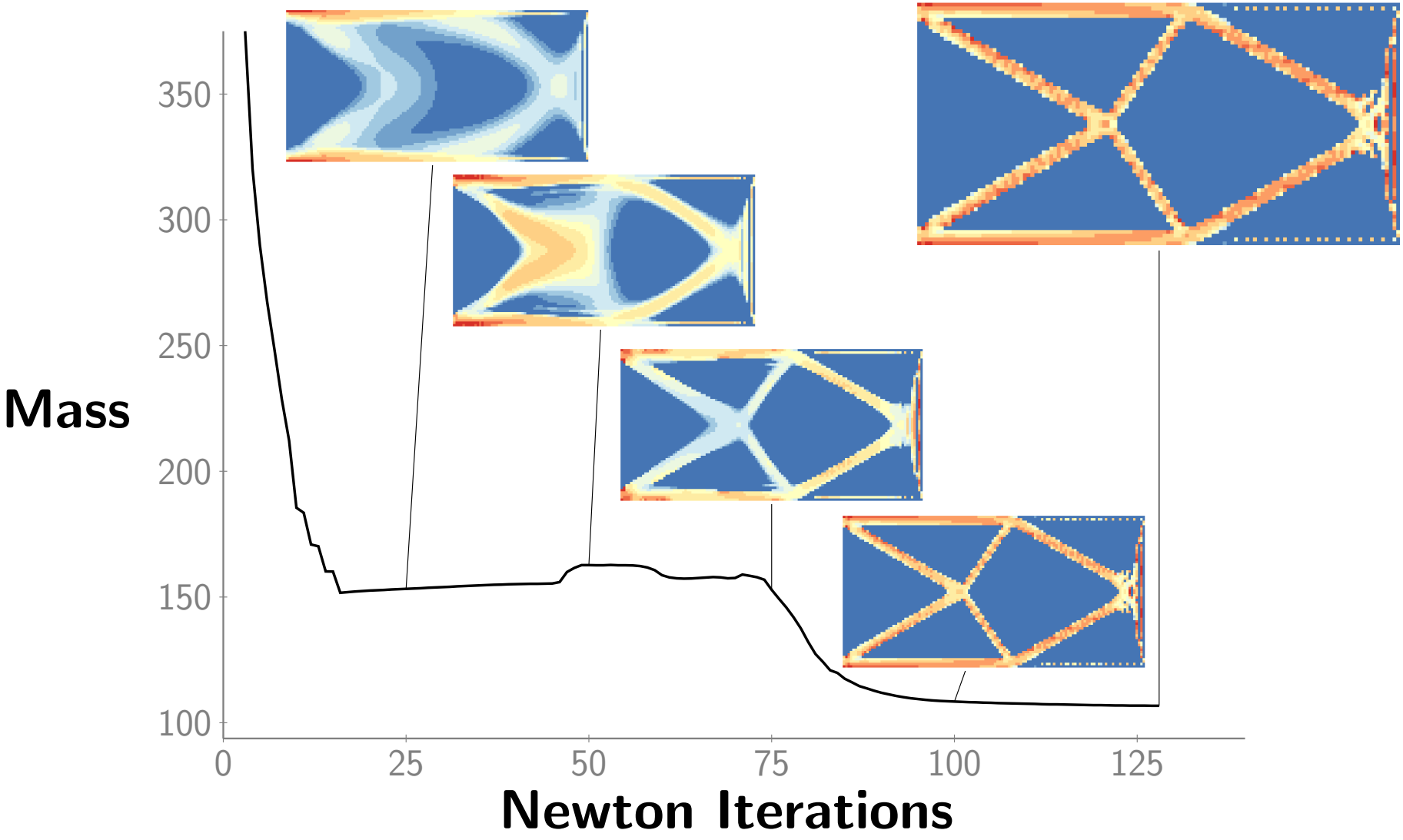
Design and stress



Topology optimization results



Topology optimization results



Conclusions

1. Large-scale topology and multimaterial problems require efficient parallel analysis, parallel gradient evaluation, and parallel optimization methods
2. Full-space barrier methods enable tailoring for specific structural optimization problems
   - Control of positive definite/indefinite terms
3. Recommendations for stress-constrained design:
   - Use direct thickness variables when performing sizing
   - Use inverse variables for topology optimization

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