Digital Engineering: Enabling Technologies to Facilitate Agile Digital Engineering Workflows

University of Missouri
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PRESENTED BY

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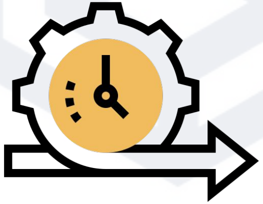
Introduction

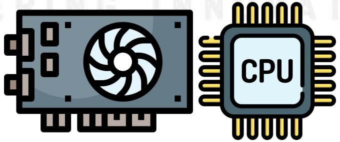
Trends



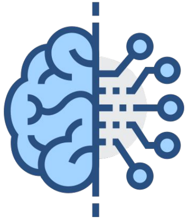
AGILE ENTERPRISE

3D PRINTING

CLOUD COMPUTING



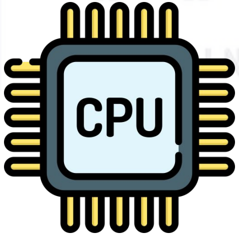
HETEROGENOUS COMPUTING



ARTIFICIAL INTELLIGENCE

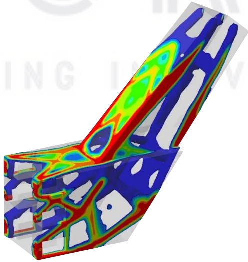
Opportunity

LEGACY
SOFTWARE



HOMOGENEOUS
COMPUTING

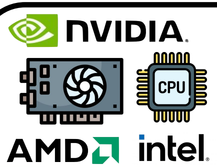
SLOW
SOFTWARE



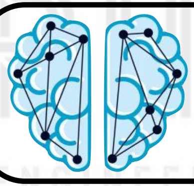
SIMPLE
SOLUTIONS

UNRELIABLE
DESIGNS

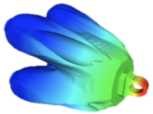
PROPOSAL



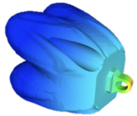
HARDWARE ABSTRACTION



INTELLIGENT DESIGN TOOL

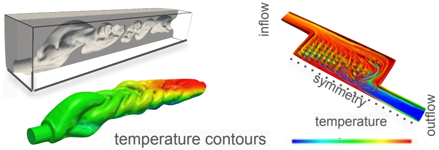


vs

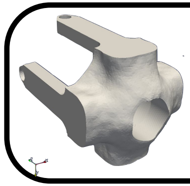


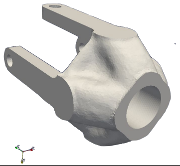
REAL-TIME DISCOVERY

Courtesy of collaborator Prof. Kurt Maute



MULTI-PHYSICS EXPLORATION

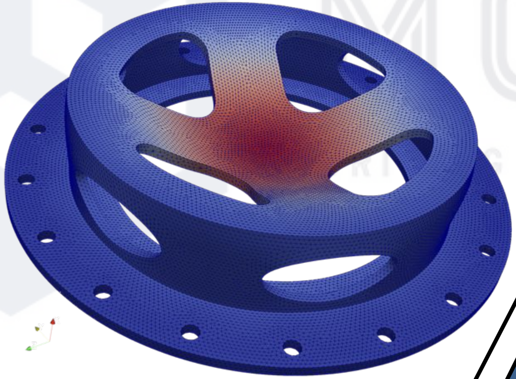


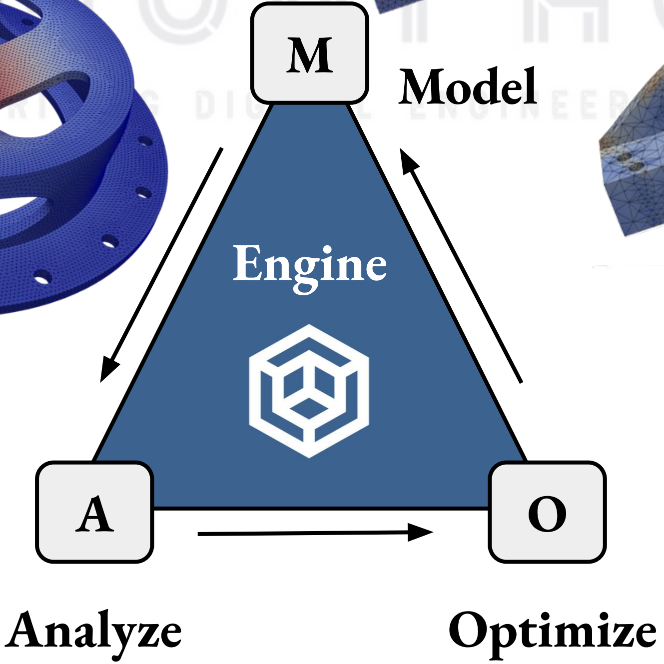


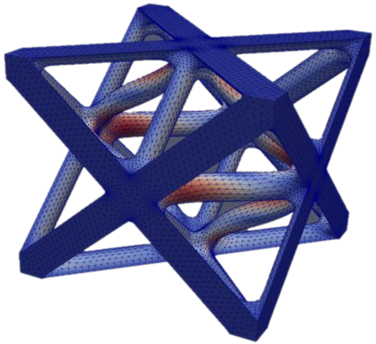
BUILT-IN RELIABILITY

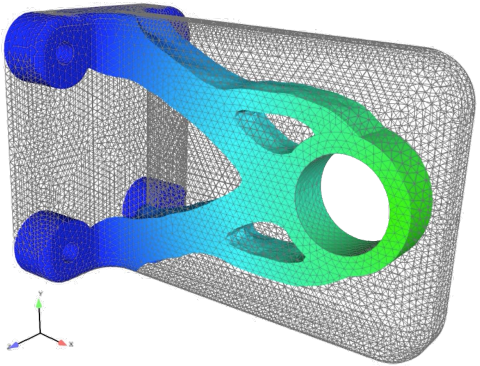
Design Platform

Design Ecosystem

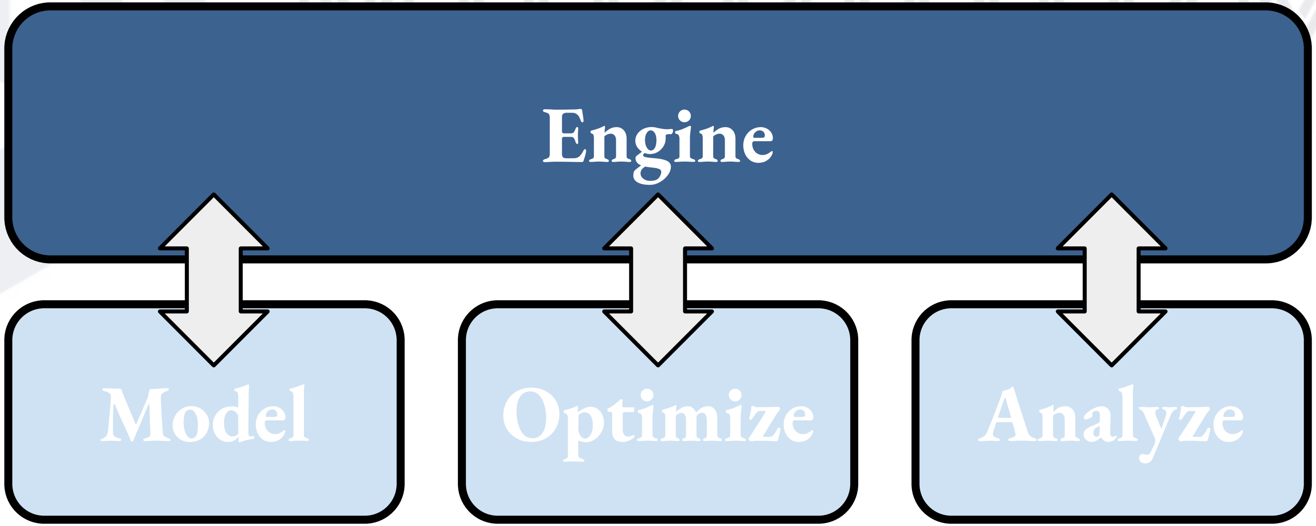






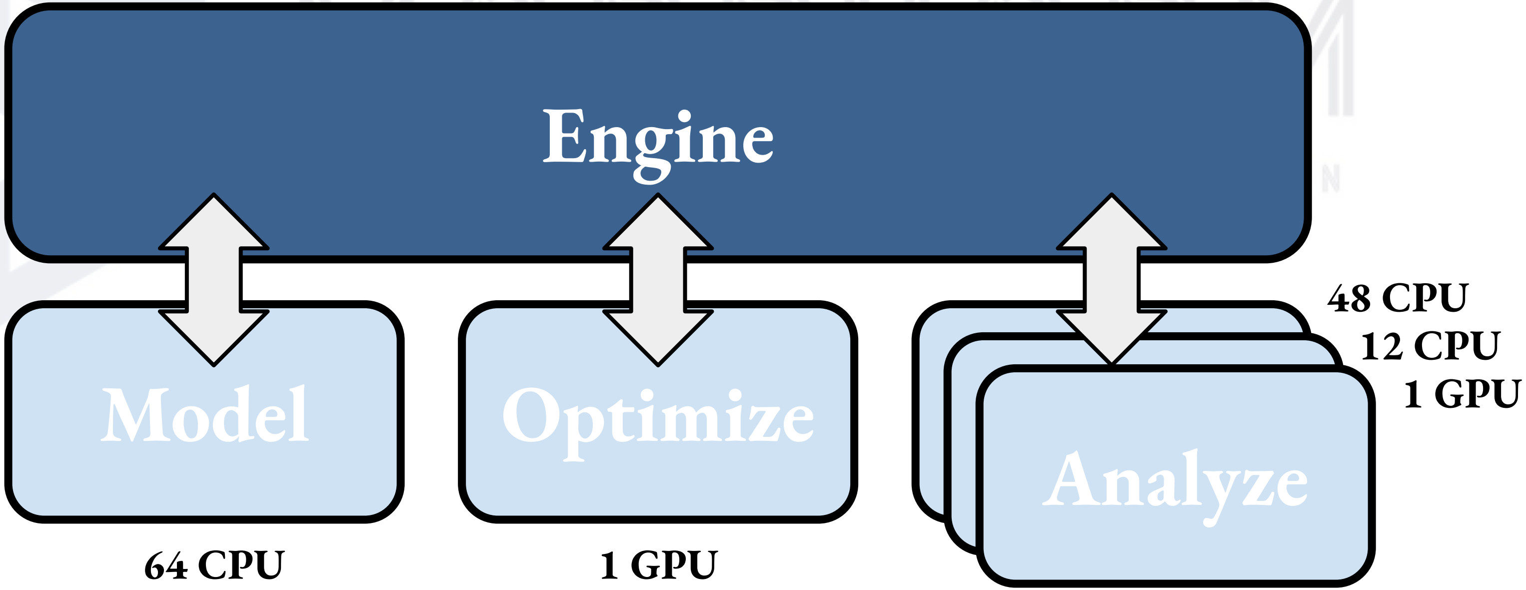


Multiple Program, Multiple Data (MPMD) Engine



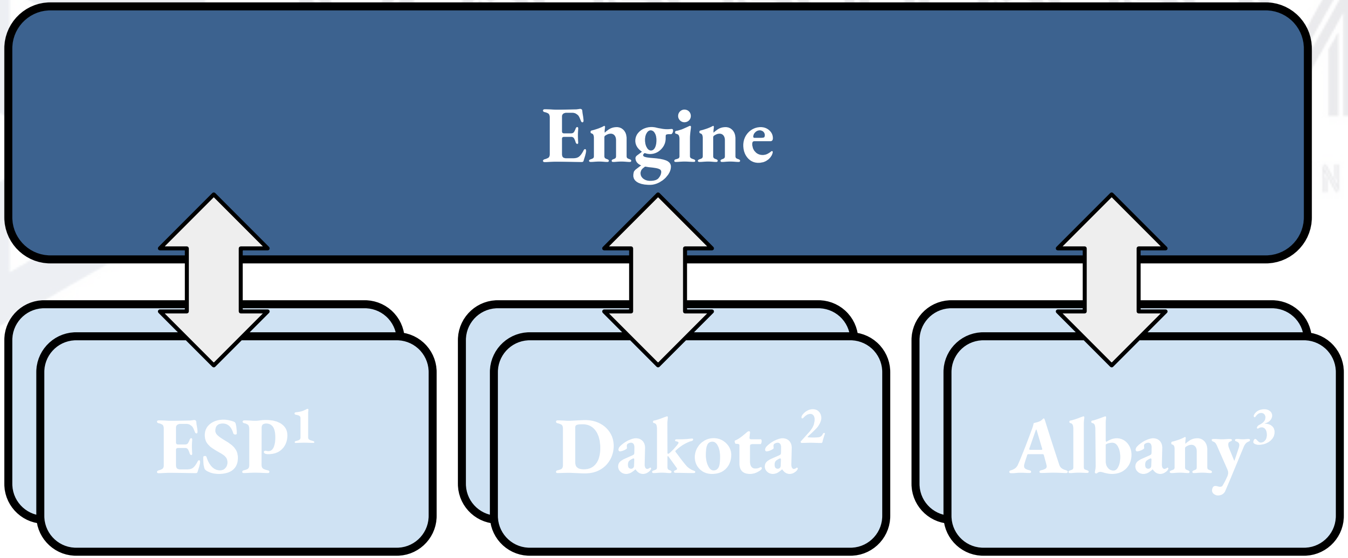
Provides automated management and execution of programs and data transfers at runtime in an HPC environment

MPMD Engine: Concurrent Evaluations



Provides automated management and execution of concurrent programs and data transfers at runtime in an HPC environment

MPMD Engine: Plug-N-Play

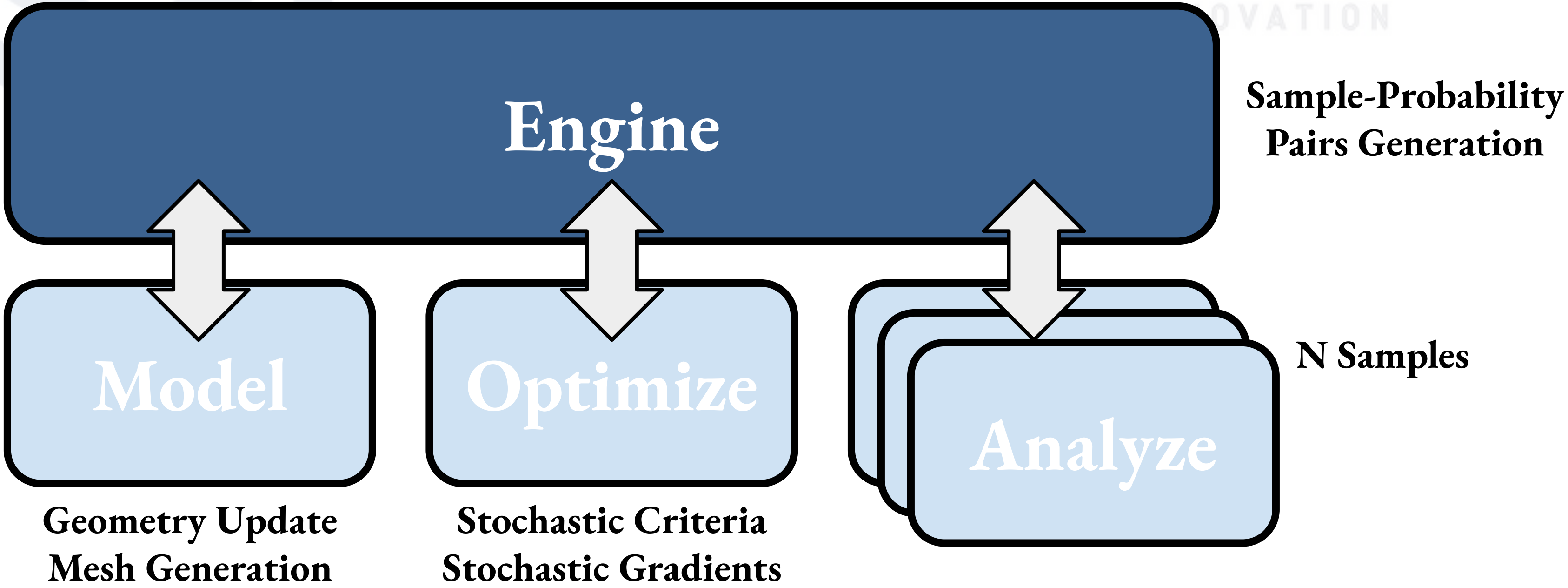


Plug new modeling, optimization, and analysis tools into the ecosystem through a simple interface

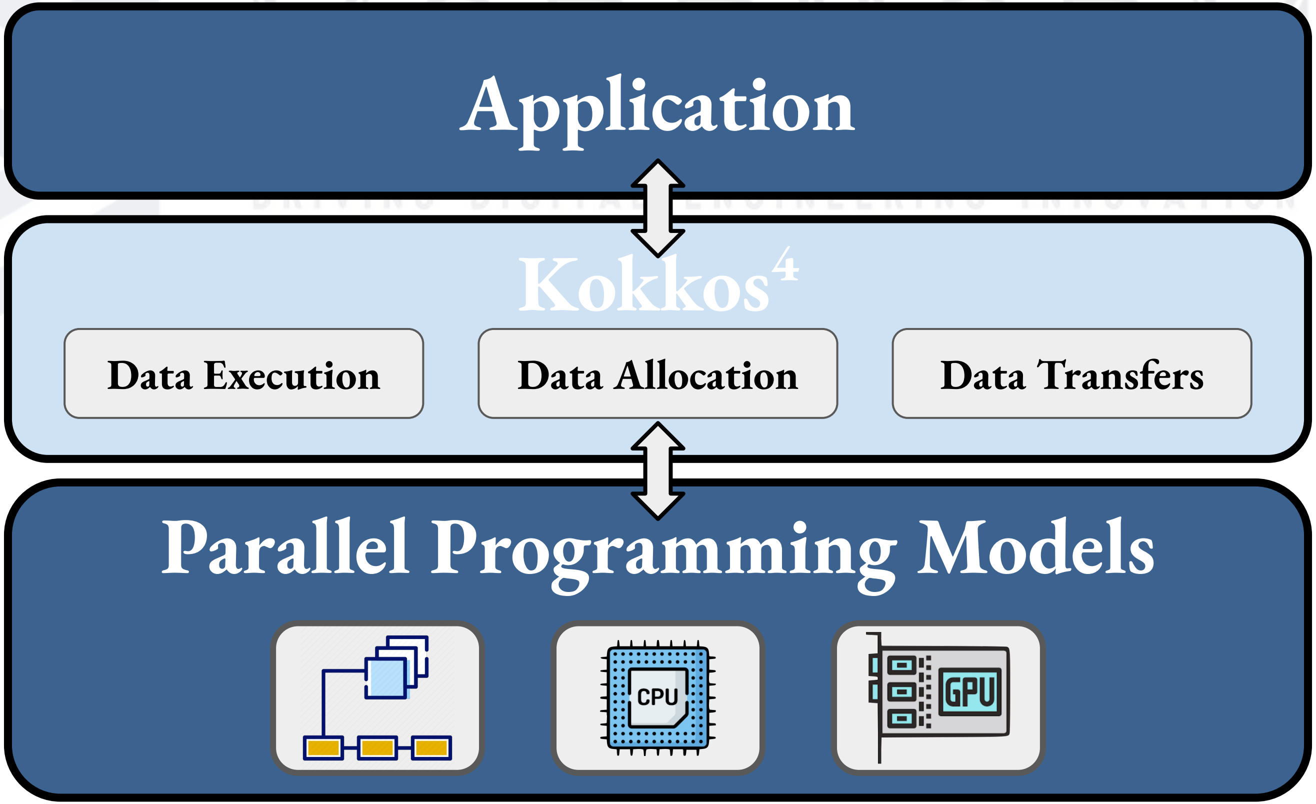
[1] https://acdl.mit.edu/ESP/ (Geometry Modeling Engine) [2] https://dakota.sandia.gov/ (Optimization & UQ Engine) [3] https://github.com/sandialabs/Albany (Multiphysics Simulation Engine)

Design Workflow Management

Problem Statement: Find the robust configuration such that the structural stiffness is improved and the mass budget is met given the input uncertainty



Performance Portability



[4] https://kokkos.org/

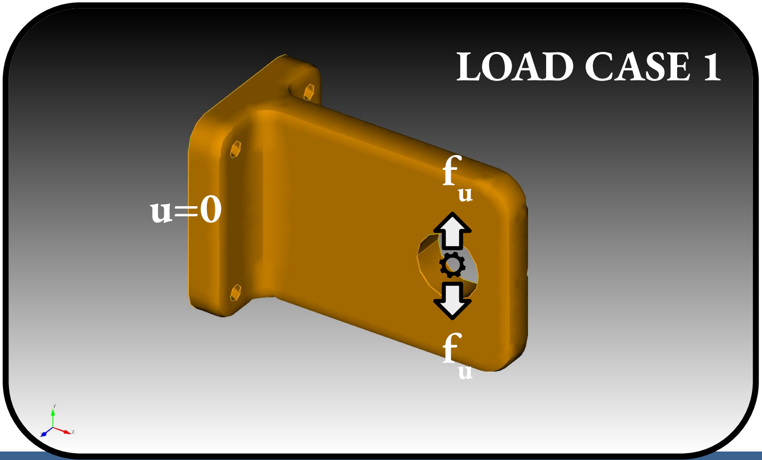
Applications

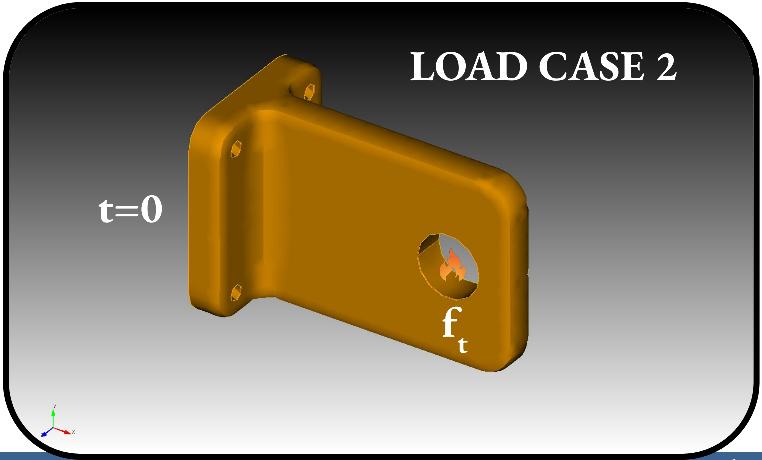
Topology Optimization

Problem Statement: Find the optimal configuration such that the structural stiffness and thermal conductivity is maximize given a mass budget

$$\min_{\mathbf{z}\in[0,1]^N} \quad f(\mathbf{z},\mathbf{u}) = \frac{\alpha_1}{2}\mathbf{u}^T\mathbf{K}_\mathbf{u}(\mathbf{z})\mathbf{u} + \frac{\alpha_2}{2}\mathbf{t}^T\mathbf{K}_\mathbf{t}(\mathbf{z})\mathbf{t} \quad \text{s.t.} \quad M(\mathbf{z}) \leq M_{lim}$$

$$\text{with:} \quad \mathbf{K}_\mathbf{u}(\mathbf{z})\mathbf{u} = \mathbf{f}_\mathbf{u} \quad \text{and} \quad \mathbf{K}_\mathbf{t}(\mathbf{z})\mathbf{t} = \mathbf{f}_\mathbf{t}$$





Total Derivative

Adjoint Method

$$\frac{df(\mathbf{z},\mathbf{u})}{d\mathbf{z}} = \frac{\partial f(\mathbf{z},\mathbf{u})}{\partial \mathbf{z}} + \xi^T \frac{\partial \mathbf{R}(\mathbf{z},\mathbf{u})}{\partial \mathbf{z}} + \underbrace{\left(\frac{\partial f(\mathbf{z},\mathbf{u})}{\partial \mathbf{u}} + \xi^T \frac{\partial \mathbf{R}(\mathbf{z},\mathbf{u})}{\partial \mathbf{u}}\right)}_{0} \frac{\partial \mathbf{u}}{\partial \mathbf{z}}$$

Adjoint Solve

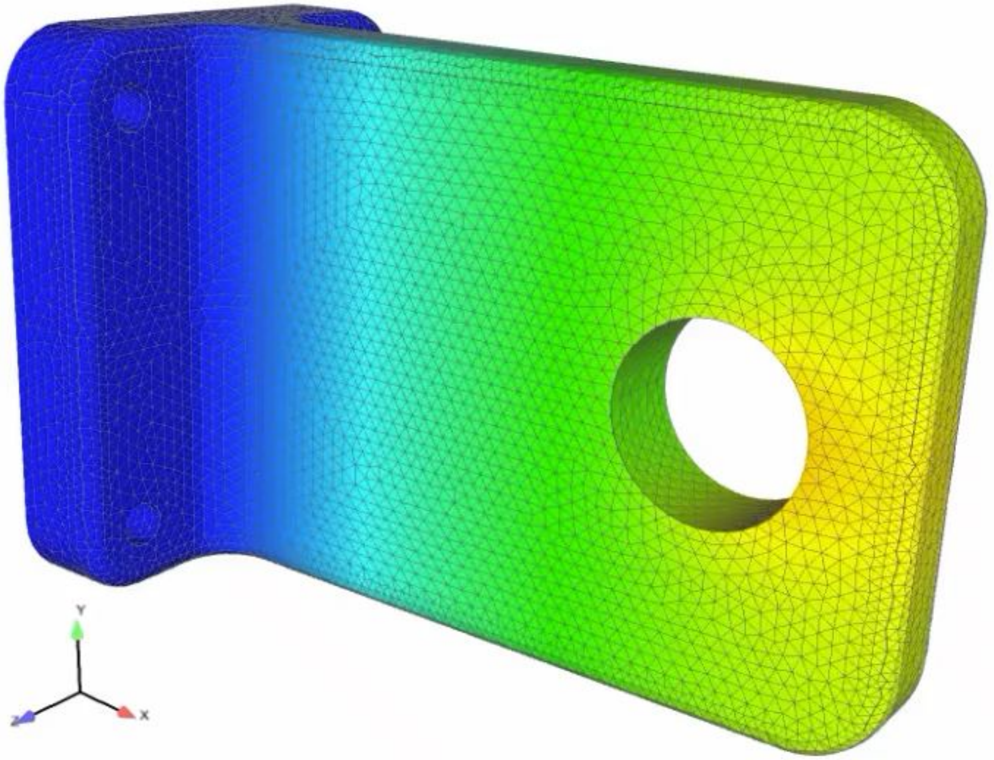
$$\xi = -\left[\left(\frac{\partial \mathbf{R}(\mathbf{z},\mathbf{u})}{\partial \mathbf{u}}\right)^T\right]^{-1} \left(\frac{\partial f(\mathbf{z},\mathbf{u})}{\partial \mathbf{u}}\right)$$

Total Derivative

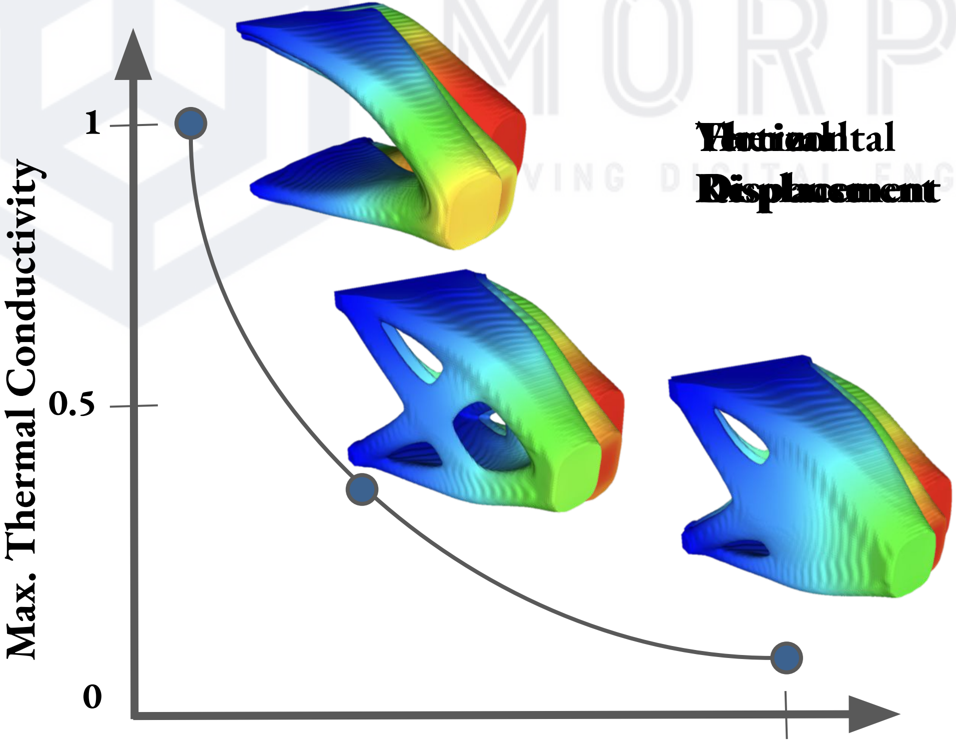
$$\frac{df(\mathbf{z},\mathbf{u})}{d\mathbf{z}} = \frac{\partial f(\mathbf{z},\mathbf{u})}{\partial \mathbf{z}} + \xi^T \frac{\partial \mathbf{R}(\mathbf{z},\mathbf{u})}{\partial \mathbf{z}}$$

Automatic Differentiation (AD) numerical methods are applied to derive the total derivative!!!

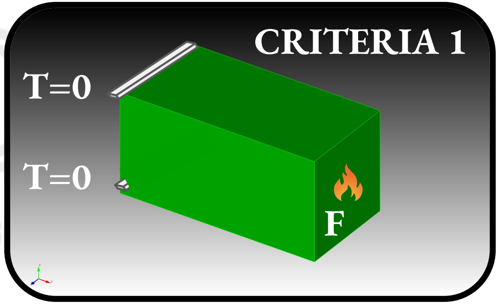
Real-Time Solution



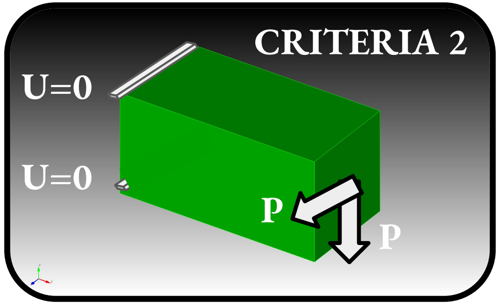
Design Exploration



Max. Structural Stiffness



Max. Thermal Conductivity



Max. Structural Stiffness

Topology Optimization

Problem Statement: Find the optimal configuration such that the structural mass is minimized and the material strength threshold is met everywhere

$$
\begin{aligned}
\min_{\mathbf{z}\in[0,1]^N} \quad & f(\mathbf{z},\mathbf{u}) = \alpha_1 M(\mathbf{z}) + \alpha_2 \mathbf{f}^T\mathbf{u} \\
\text{s.t.} \quad & g_j(\mathbf{z},\mathbf{u}) \leq 0 \quad 0,\ldots,j \\
\text{with:} \quad & \mathbf{K}(\mathbf{z})\,\mathbf{u} = \mathbf{f}
\end{aligned}
$$

where

$$
g_j(\mathbf{z},\mathbf{u}) = P_j(\mathbf{z})\Lambda_j\left(\Lambda_j^2+1\right) \leq 0 \qquad \Lambda_j = \sigma_j^{vm}/\sigma_{lim} - 1
$$

Constraints need to be handled with care to avoid a computationally intensive solution method

Augmented Lagrangian (AL) Method[5]

The optimization problem formulation defined on slide 6 is recast as the solution of a sequence of optimization problems aiming to minimize the AL function:

$$\min_{\mathbf{z}\in[0,1]^N} \quad J^{(k)}(\mathbf{z},\mathbf{u}) = f(\mathbf{z},\mathbf{u}) + \frac{1}{N}\sum_{j=1}^{N}\left[\lambda_j^{(k)} h_j(\mathbf{z},\mathbf{u}) + \frac{\mu^{(k)}}{2} h_j(\mathbf{z},\mathbf{u})^2\right]$$

where

$$h_j(\mathbf{z},\mathbf{u}) = \max\left(g_j(\mathbf{z},\mathbf{u}), -\frac{\lambda_j^{(k)}}{\mu_j^{(k)}}\right)$$ Constraint Evaluation

$$\lambda_j^{(k+1)} = \lambda_j^{(k+1)} + \mu_j^{(k)} h_j(\mathbf{z},\mathbf{u})$$ Lagrange Multiplier

$$\min\left(\beta\mu_j^{(k)}, \mu_{\max}\right), \ \beta > 1$$ Penalty Update

[5]O. Giraldo-Londono, J.B. Russ, M.A. Aguilo, and G.H. Paulino, "Limiting the first principal stress in topology optimization: A local and consistent approach", Structural and Multidisciplinary Optimization 2022

Total Derivative

Adjoint Method

$$\frac{dJ^{(k)}(\mathbf{z},\mathbf{u})}{d\mathbf{z}} = \frac{\partial J^{(k)}(\mathbf{z},\mathbf{u})}{\partial \mathbf{z}} + \xi^T \frac{\partial \mathbf{R}^{(k)}(\mathbf{z},\mathbf{u})}{\partial \mathbf{z}} + \underbrace{\left(\frac{\partial J^{(k)}(\mathbf{z},\mathbf{u})}{\partial \mathbf{u}} + \xi^T \frac{\partial \mathbf{R}^{(k)}(\mathbf{z},\mathbf{u})}{\partial \mathbf{u}} \right)}_{0} \frac{\partial \mathbf{u}}{\partial \mathbf{z}}$$

Adjoint Solve

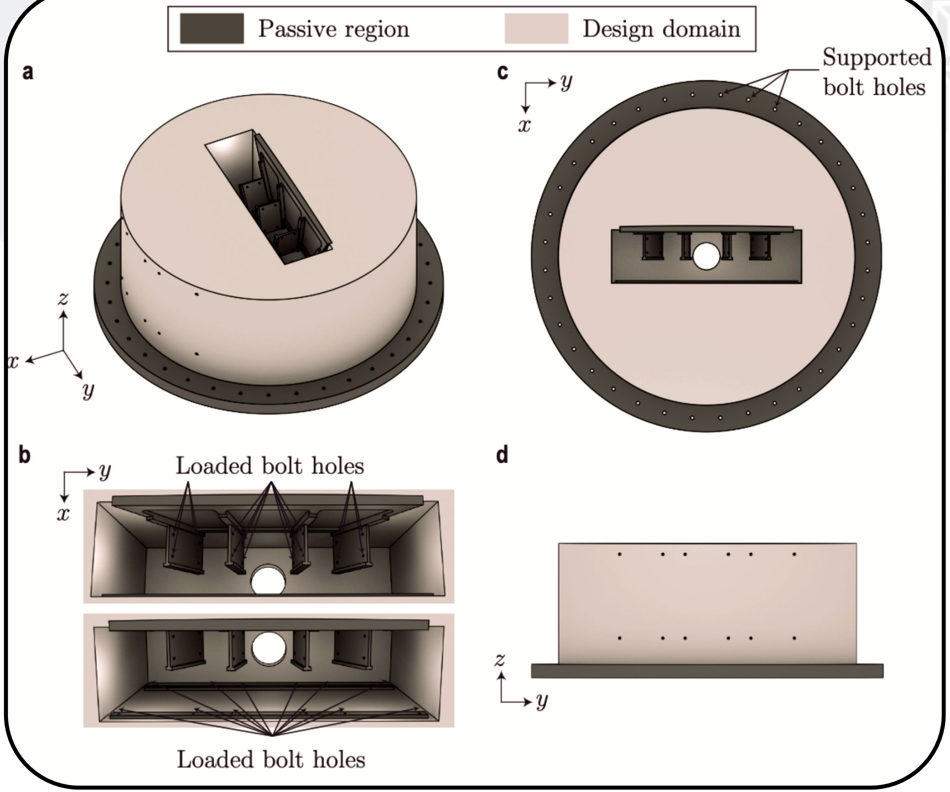
$$\xi^{(k)} = -\left[\left(\frac{\partial \mathbf{R}^{(k)}(\mathbf{z},\mathbf{u})}{\partial \mathbf{u}} \right)^T \right]^{-1} \left(\frac{\partial J^{(k)}(\mathbf{z},\mathbf{u})}{\partial \mathbf{u}} \right)$$

Only One Adjoint Solve Per AL Iteration!!!

Total Derivative

$$\frac{dJ^{(k)}(\mathbf{z},\mathbf{u})}{d\mathbf{z}} = \frac{\partial J^{(k)}(\mathbf{z},\mathbf{u})}{\partial \mathbf{z}} + \left(\xi^{(k)}\right)^T \frac{\partial \mathbf{R}^{(k)}(\mathbf{z},\mathbf{u})}{\partial \mathbf{z}}$$

Example



Problem Statement: Find the optimal configuration such that the structural mass is minimized and the material strength threshold is met everywhere

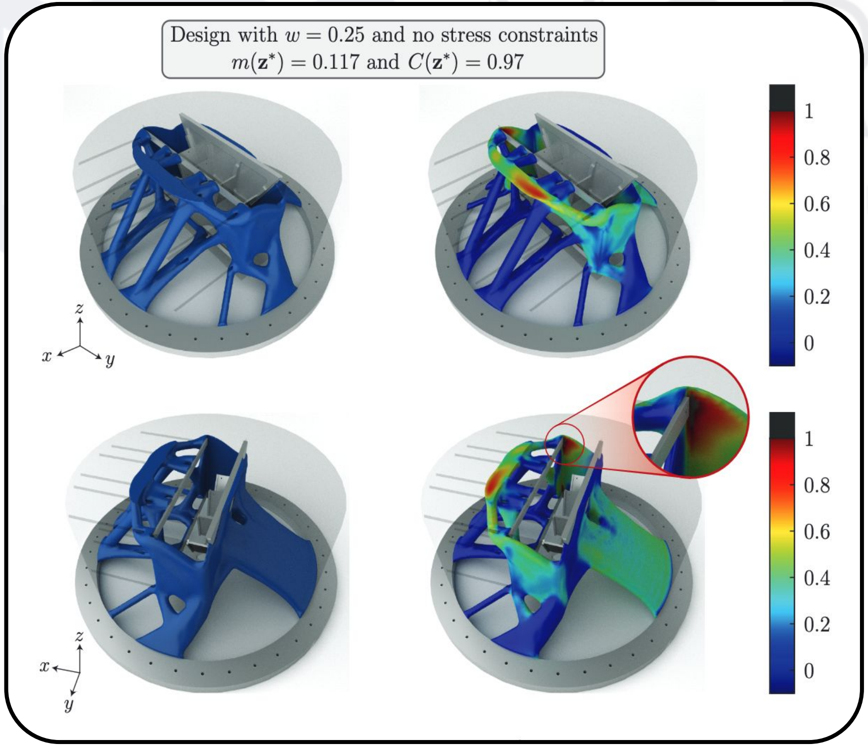
Problem Setup

Linear Elasticity

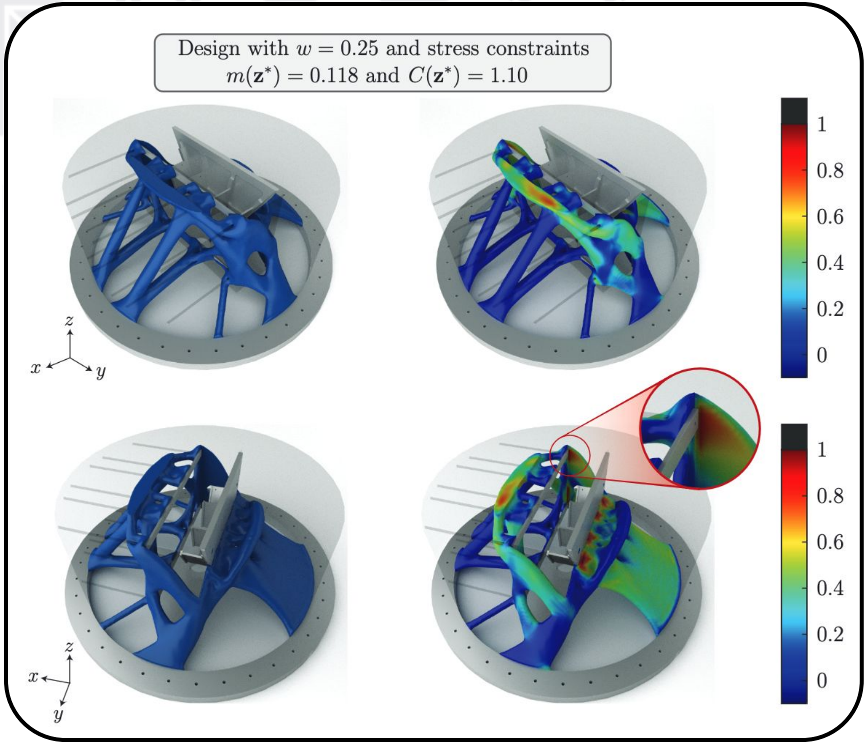
- Young's Modulus: 70 GPa
- Poisson's Ratio: 0.33

Traction Load: $\{1\text{x}10^3, 0.05\text{x}10^3, 0.05\text{x}10^3\}$
Stress Limit: 140 MPa

Results



Without Stress Constraints



With Stress Constraints

Design Under Uncertainty

Problem Statement: Find the robust configuration such that the structural stiffness is improved and the mass budget is met given the input uncertainty

$$\begin{aligned} \min_{\mathbf{z}\in[0,1]^N} \quad & \mathcal{J}\left(\mathbf{z},\mathbf{U};\Theta\right) = \mathbb{E}\left[\mathbf{C}(\mathbf{z},\mathbf{U};\Theta)\right] + \kappa \mathrm{Std}\left[\mathbf{C}(\mathbf{z},\mathbf{U};\Theta)\right] \\ \text{s.t.} \quad & M(\mathbf{z}) \leq M_{lim} \\ \text{with:} \quad & \mathbf{K}(\mathbf{z};\Theta)\mathbf{U} = \mathbf{F}(\Theta) \end{aligned}$$

where

$$\mathbf{C}(\mathbf{z},\mathbf{U};\Theta) = \alpha \mathbf{F}(\Theta)^T \mathbf{U}(\mathbf{z};\Theta)$$

Structural Compliance

The goal is to find a robust configuration over all the expected environments

Approximation

Robust Optimization Formulation

$$\min_{\mathbf{z}\in[0,1]^N} \quad \widehat{\mathcal{J}}\left(\mathbf{z},\mathbf{U};\Theta\right) = \widehat{\mathbb{E}}\left[\mathbf{C}(\mathbf{z},\mathbf{U};\Theta)\right] + \kappa\widehat{\mathrm{Std}}\left[\mathbf{C}(\mathbf{z},\mathbf{U};\Theta)\right]$$

$$\text{s.t.} \quad M(\mathbf{z}) \leq M_{lim}$$

$$\text{with:} \quad \widehat{\mathbf{K}}(\mathbf{z};\theta^{(j)})\widehat{\mathbf{U}}^{(j)} = \widehat{\mathbf{F}}(\theta^{(j)}) \quad \text{for} \quad j = 1,\cdots,N_s$$

Adjoint Solve

$$\frac{d\widehat{J}^{(j)}}{d\mathbf{z}} = \frac{\partial\widehat{J}^{(j)}}{\partial\mathbf{z}} + \left(\xi^{(j)}\right)^T\frac{\partial\mathbf{R}^{(j)}}{\partial\mathbf{z}} + \underbrace{\left(\frac{\partial\widehat{J}^{(j)}}{\partial\widehat{\mathbf{U}}^{(j)}} + (\xi^{(j)})^T\frac{\partial\mathbf{R}^{(j)}}{\partial\widehat{\mathbf{U}}^{(j)}}\right)}_{0}\frac{\partial\widehat{\mathbf{U}}^{(j)}}{\partial\mathbf{z}} \Longrightarrow \underbrace{\xi^{(j)} = -\left[\left(\frac{\partial\mathbf{R}^{(j)}}{\partial\widehat{\mathbf{U}}^{(j)}}\right)^T\right]^{-1}\left(\frac{\partial\widehat{J}^{(j)}}{\partial\widehat{\mathbf{U}}^{(j)}}\right)}_{\text{adjoint solve}}$$

Stochastic Total Derivative

$$\frac{d\widehat{J}^{(j)}}{d\mathbf{z}} = \frac{\partial\widehat{J}^{(j)}}{\partial\mathbf{z}} + \left(\xi^{(j)}\right)^T\frac{\partial\mathbf{R}^{(j)}}{\partial\mathbf{z}}$$

Monte Carlo Method

Expectation

$$\widehat{\mathbb{E}}\left[\mathbf{C}\right] = \widehat{\mathbb{E}}\left[\mathbf{C}(\mathbf{z}, \mathbf{U}; \Theta)\right] = \frac{1}{N_s}\sum_{j=1}^{N_s}\left(\widehat{\mathbf{c}}(\mathbf{z}, \widehat{\mathbf{U}}^{(j)}; \theta^{(j)})\right) = \frac{1}{N_s}\sum_{j=1}^{N_s}\left(\widehat{\mathbf{c}}^{(j)}\right)$$

Standard Deviation

$$\widehat{\mathrm{Std}}\left[\mathbf{C}(\mathbf{z}, \mathbf{U}; \Theta)\right] = \sqrt{\widehat{\mathbb{E}}\left[\mathbf{C}^2\right] + \widehat{\mathbb{E}}\left[\mathbf{C}\right]^2} = \sqrt{\frac{1}{N_s}\sum_{j=1}^{N_s}\left(\widehat{\mathbf{c}}^{(j)}\right)^2 - \left(\frac{1}{N_s}\sum_{j=1}^{N_s}\widehat{\mathbf{c}}^{(j)}\right)^2}$$

Stochastic Total Derivative

$$\frac{d\widehat{J}}{d\mathbf{z}} = \frac{1}{N_s}\sum_{j=1}^{N_s}\left[\left(1 + \kappa\frac{\widehat{\mathbf{c}}^{(j)} - \mathbb{E}\left[\mathbf{C}\right]}{\mathrm{Std}\left[\mathbf{C}\right]}\right)\frac{\partial\widehat{\mathbf{c}}^{(j)}}{\partial\mathbf{z}}\right]$$

Stochastic Reduced Order Model (SROM) Method[6]

Expectation

$$\widehat{\mathbb{E}}\left[\mathbf{C}\right] = \widehat{\mathbb{E}}\left[\mathbf{C}(\mathbf{z}, \mathbf{U}; \Theta)\right] = \sum_{j=1}^{M_s} \widehat{\mathbf{c}}(\mathbf{z}, \widehat{\mathbf{U}}^{(j)}; \theta^{(j)}) p^{(j)} = \sum_{j=1}^{M_s} \widehat{\mathbf{c}}^{(j)} p^{(j)}$$

Standard Deviation

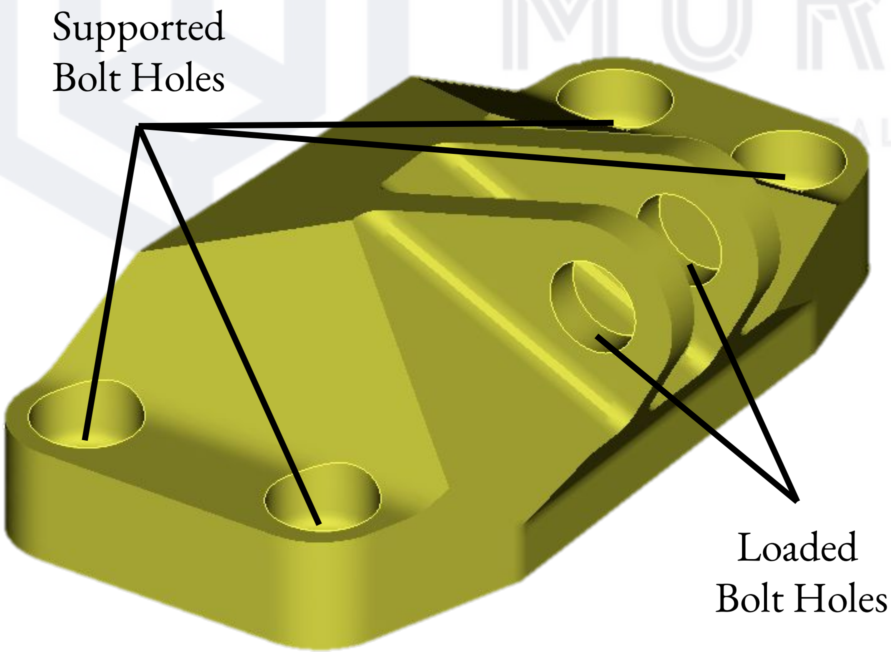
$$\widehat{\mathrm{Std}}\left[\mathbf{C}(\mathbf{z}, \mathbf{U}; \Theta)\right] = \sqrt{\widehat{\mathbb{E}}\left[\mathbf{C}^2\right] + \widehat{\mathbb{E}}\left[\mathbf{C}\right]^2} = \sqrt{\sum_{j=1}^{M_s} \left(\widehat{\mathbf{c}}^{(j)}\right)^2 p^{(j)} - \left(\sum_{j=1}^{M_s} \widehat{\mathbf{c}}^{(j)} p^{(j)}\right)^2}$$

Stochastic Total Derivative

$$\frac{d\widehat{J}}{d\mathbf{z}} = \sum_{j=1}^{M_s} \left[p^{(j)} \left(1 + \kappa \frac{\widehat{\mathbf{c}}^{(j)} - \mathbb{E}\left[\mathbf{C}\right]}{\mathrm{Std}\left[\mathbf{C}\right]} \right) \frac{\partial \widehat{\mathbf{c}}^{(j)}}{\partial \mathbf{z}} \right]$$

[6] Torres, A. P., Warner, J. E., Aguiló, M. A., & Guest, J. K. (2021). Robust topology optimization under loading uncertainties via stochastic reduced order models. *IJNME*, *122*(20), 5718-5743.

Example



Problem Statement: Find the robust configuration such that the structural stiffness is improved and the mass budget is met given the input material and load uncertainties.

Problem Setup

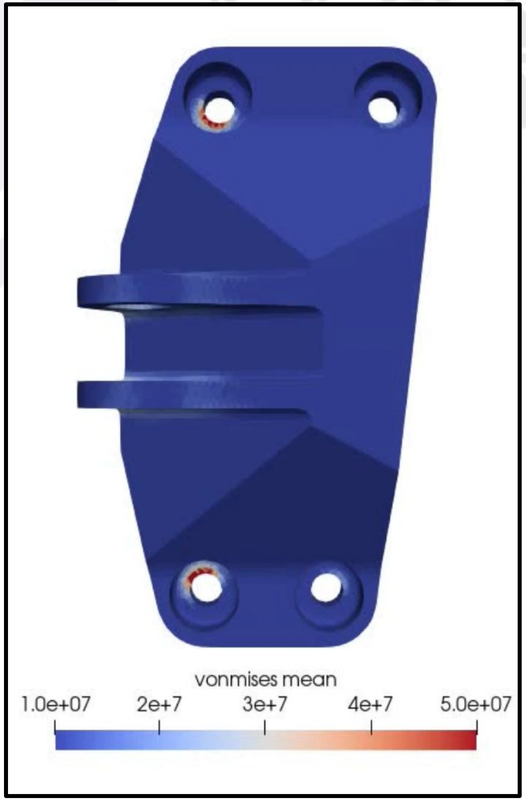
Linear Elasticity

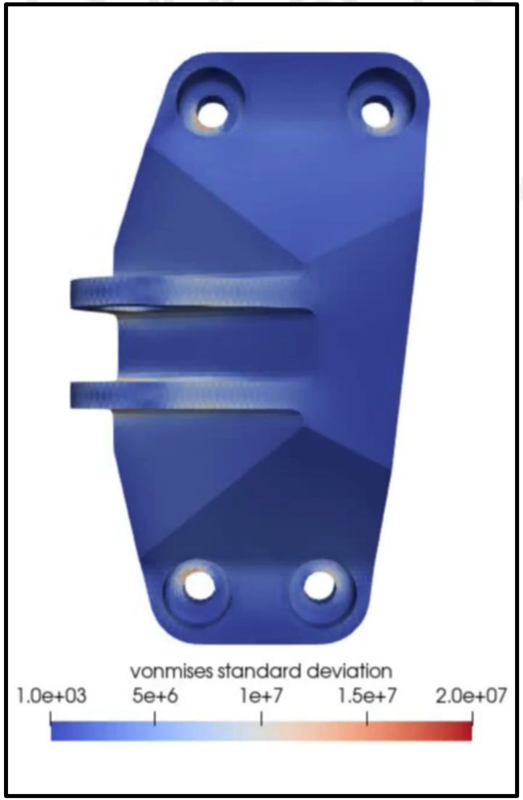
- Young's Modulus: *N*(70 GPa,10 GPa)
- Poisson's Ratio: 0.33

Traction Load: {*N*(1 KPa,0.1 KPa), {N(0.5 KPa,0.2 KPa), *N*(0.5 KPa,0.25 KPa)}

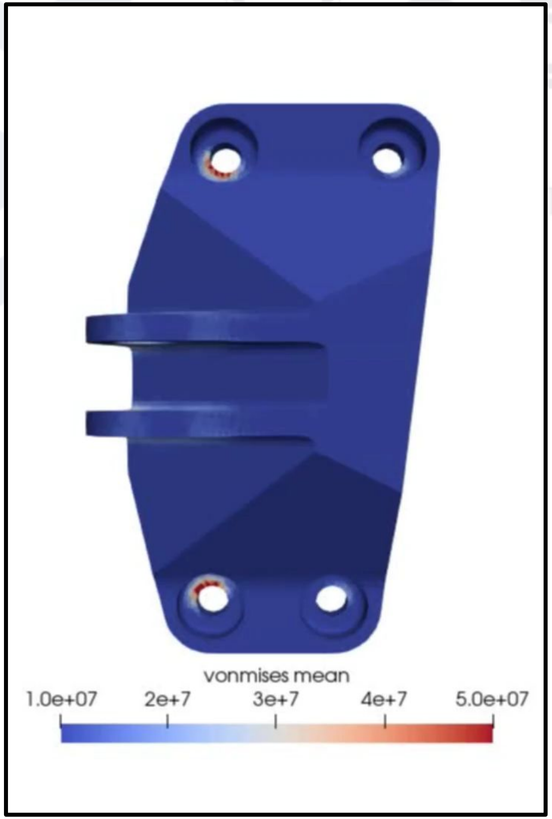
Stress Limit: 140 MPa

Results: Structural Topology Optimization



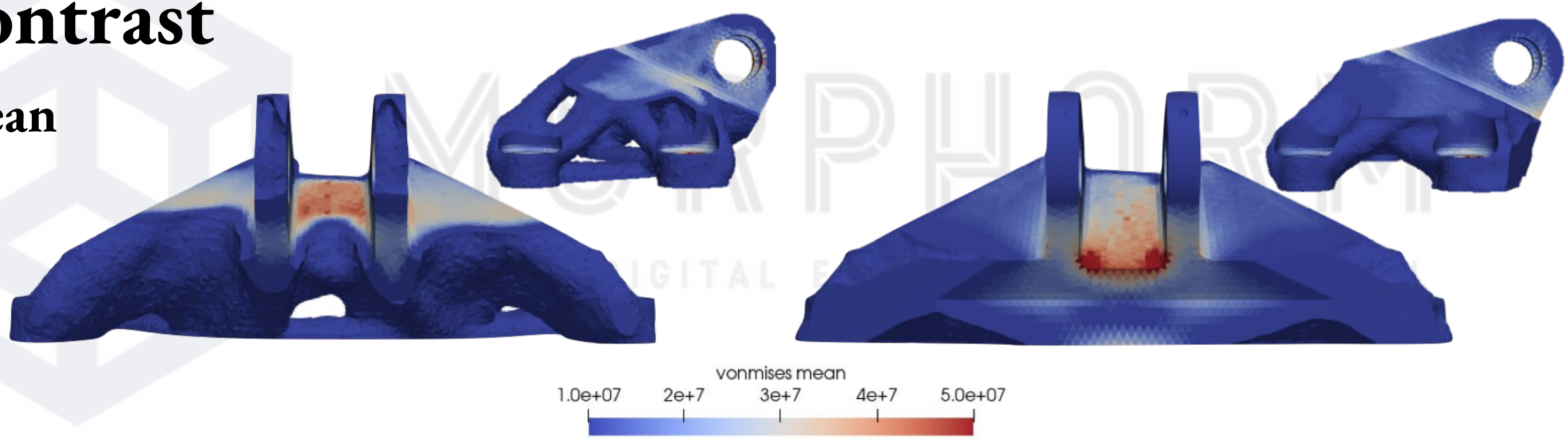


Results: Meet Material Strength Threshold

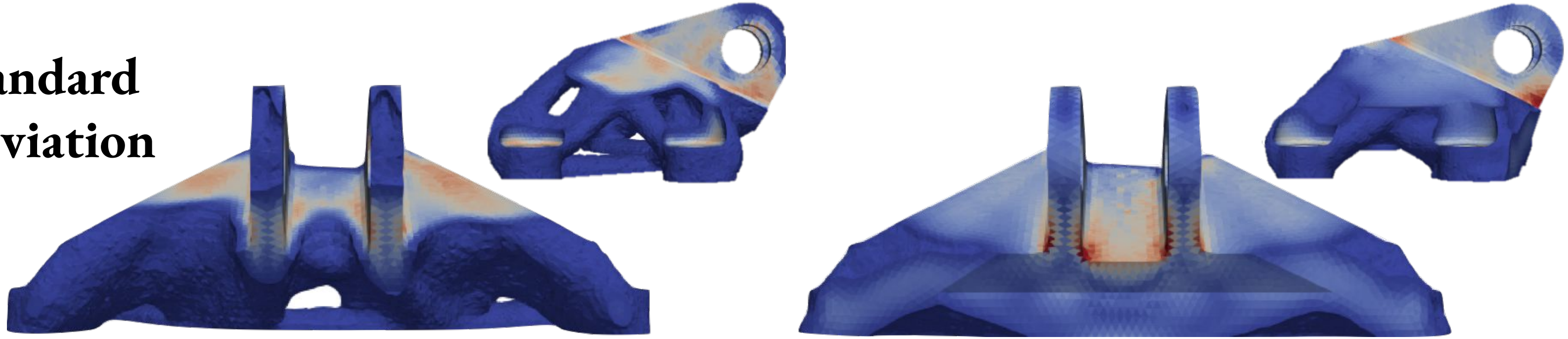


Contrast

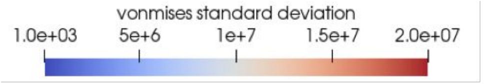
Mean



Standard Deviation



Stress-Based Design



Stiffness-Based Design

Computational Fluid Dynamics

Problem Statement: Find the flow channel configuration that minimizes the pressure difference between fluid inlet and outlet given a mass budget.

$$\min_{\mathbf{z}\in[0,1]^N} \quad \frac{\alpha}{2}\|\mathbf{p}_{in} - \mathbf{p}_{out}\|^2$$

$$\text{s.t.} \quad M(\mathbf{z}) \leq M_{lim}$$

$$\text{with:} \quad \frac{\partial \mathbf{u}_i}{\partial \mathbf{x}_i} = 0$$

Incompressibility Condition

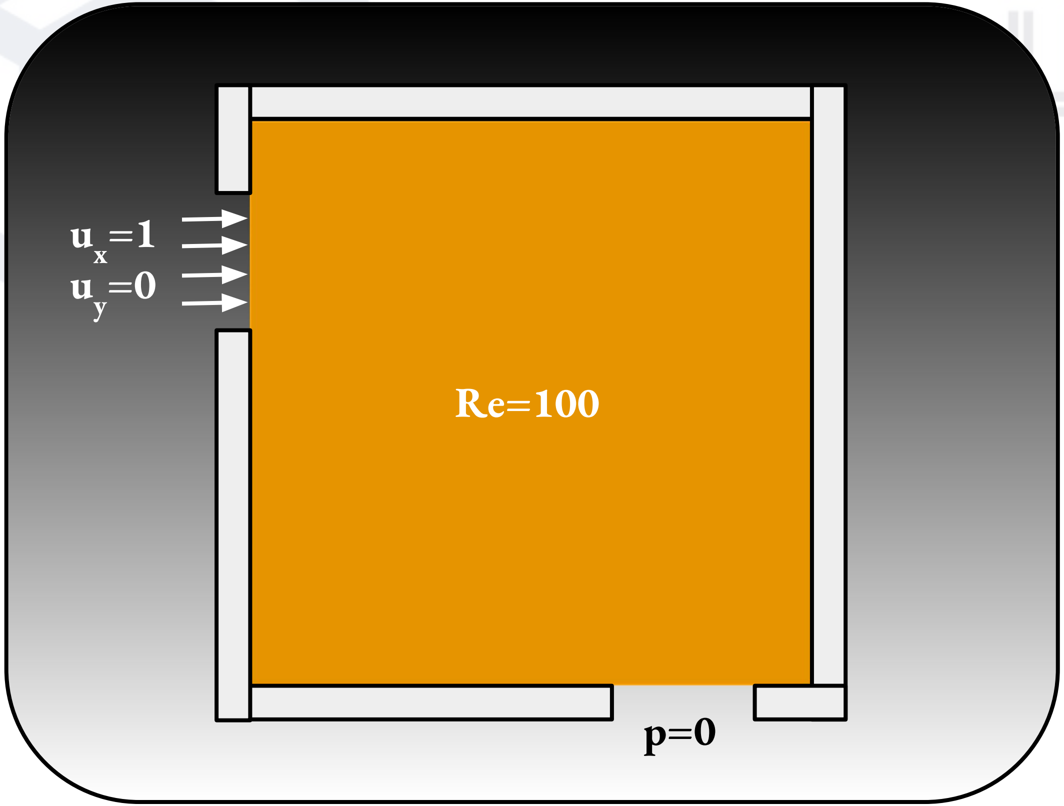
$$\frac{1}{c^2}\frac{\partial \mathbf{p}}{\partial t} = -\rho_0 \frac{\partial \mathbf{u}_i}{\partial \mathbf{x}_i} \quad \text{in} \quad \Omega$$

Conservation of Mass

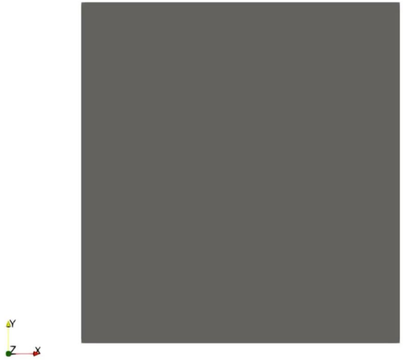
$$\rho_0 \left[\frac{\partial \mathbf{u}_i}{\partial t} + \frac{\partial}{\partial \mathbf{x}_j}(\mathbf{u}_i \mathbf{u}_j)\right] = -\frac{\partial \mathbf{p}}{\mathbf{x}_i} + \frac{\partial \tau_{ij}}{\partial \mathbf{x}_j} \quad \text{in} \quad \Omega$$

Conservation of Momentum

Results



Problem Statement: Find the best flow channel configuration that minimizes the pressure difference between fluid inlet and outlet given a mass budget.

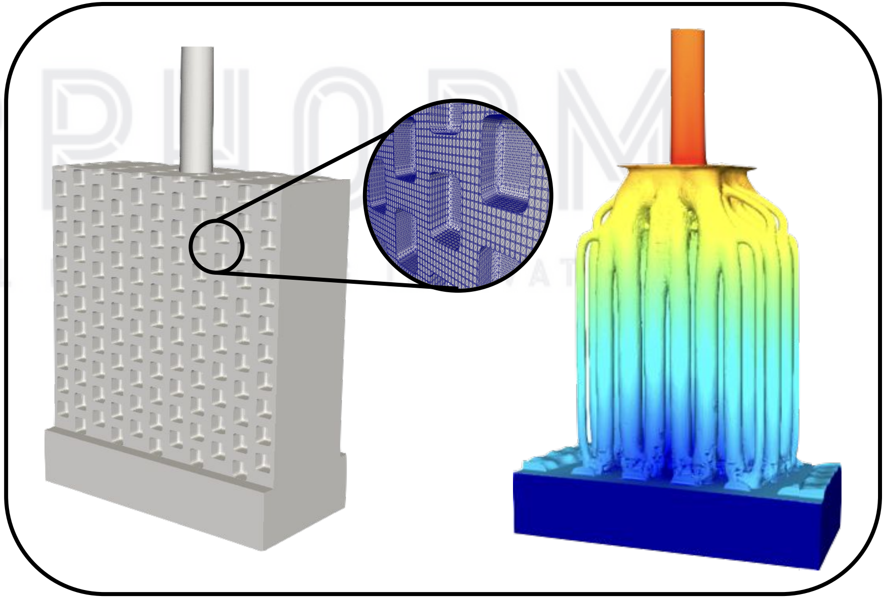


Fluid Velocity Field

Final Thoughts

Conclusions

- Model-based design is intrinsically complex and multiphysics
- Automated management of software interactions is mandatory to effectively solve design problems driven by analysis and optimization
- Performance portability extends the lifespan of software products for digital engineering and scientific computing



Problem Statement[7]: Find the geometry of flow channels that minimize the outer surface temperature for a given pressure difference between fluid reservoir and outlet.

[7] Partnership with Prof. Kurt Maute at University of Colorado Boulder

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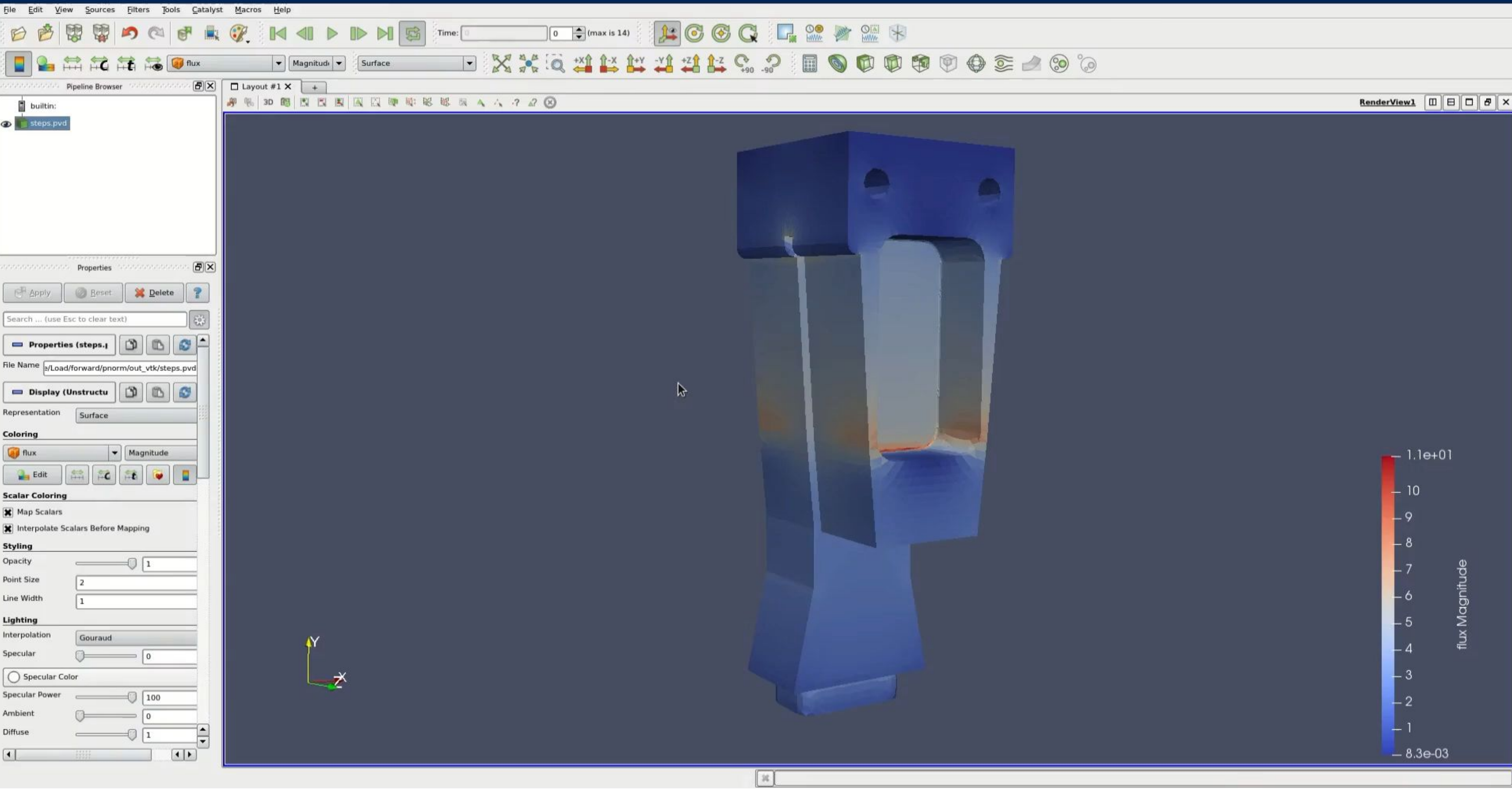
DRIVING DIGITAL ENGINEERING INNOVATION

Thank you for your time

info@morphorm.com

Backups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