Digital Engineering: Enabling Technologies to Facilitate Agile Digital Engineering Workflows

University of New Mexico
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PRESENTED BY

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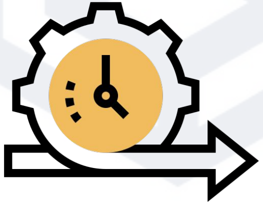
Introduction

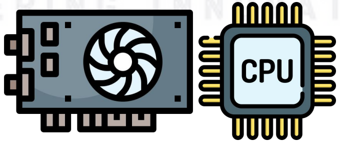
Trends



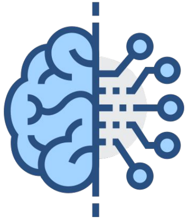
AGILE ENTERPRISE

3D PRINTING

CLOUD COMPUTING



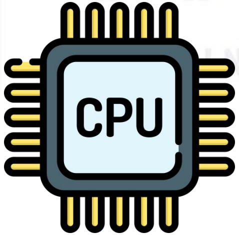
HETEROGENOUS COMPUTING



ARTIFICIAL INTELLIGENCE

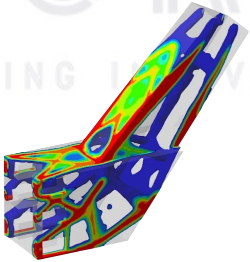
Opportunity

LEGACY
SOFTWARE



HOMOGENEOUS
COMPUTING

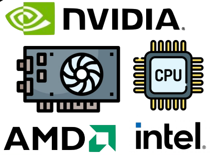
SLOW
SOFTWARE



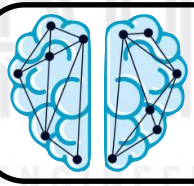
SIMPLE
SOLUTIONS

UNRELIABLE
DESIGNS

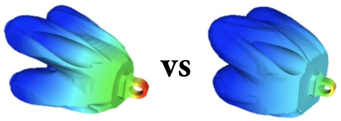
PROPOSAL



HARDWARE ABSTRACTION

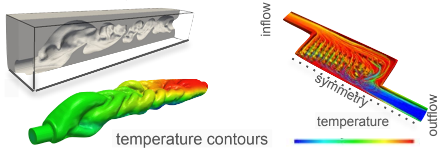


INTELLIGENT DESIGN TOOL

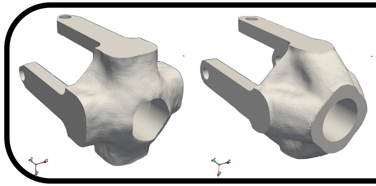


REAL-TIME DISCOVERY

Courtesy of collaborator Prof. Kurt Maute



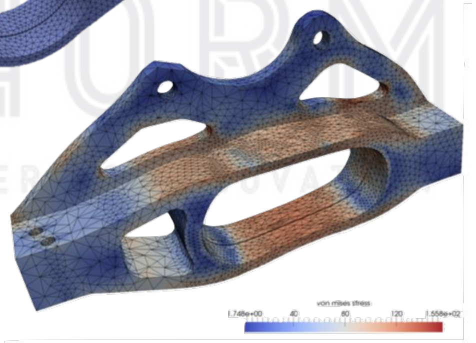
MULTI-PHYSICS EXPLORATION

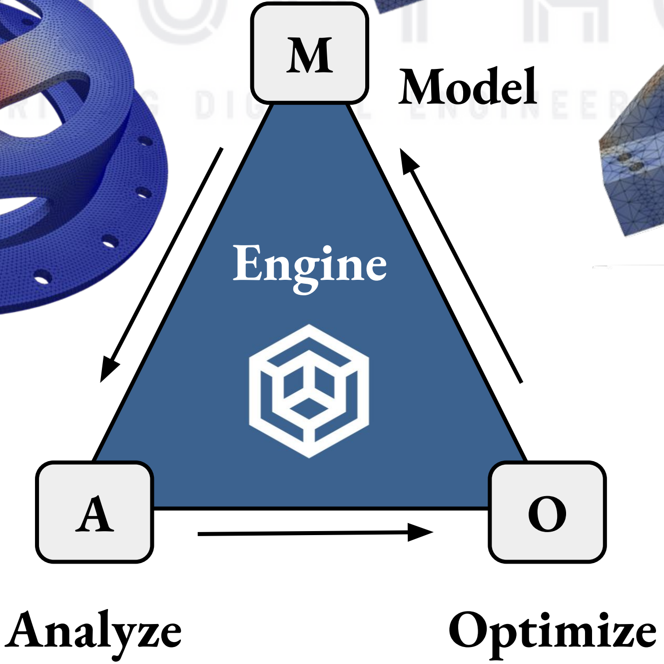


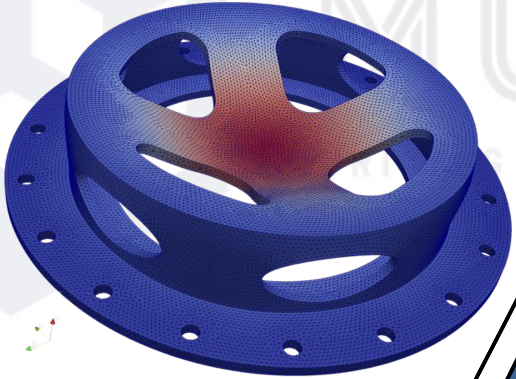
BUILT-IN RELIABILITY

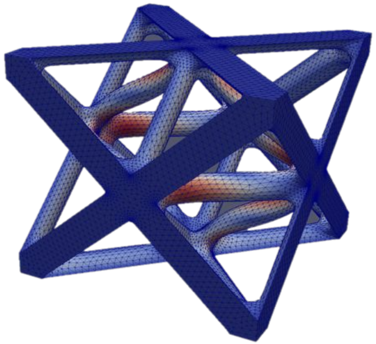
Design Platform

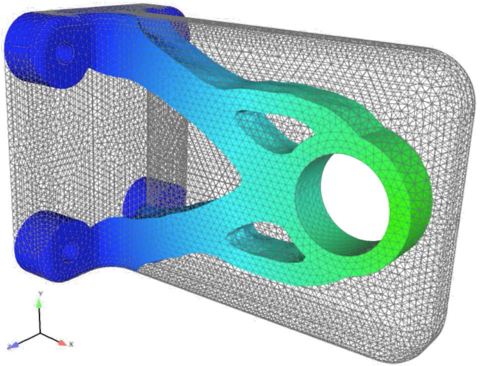
Design Ecosystem



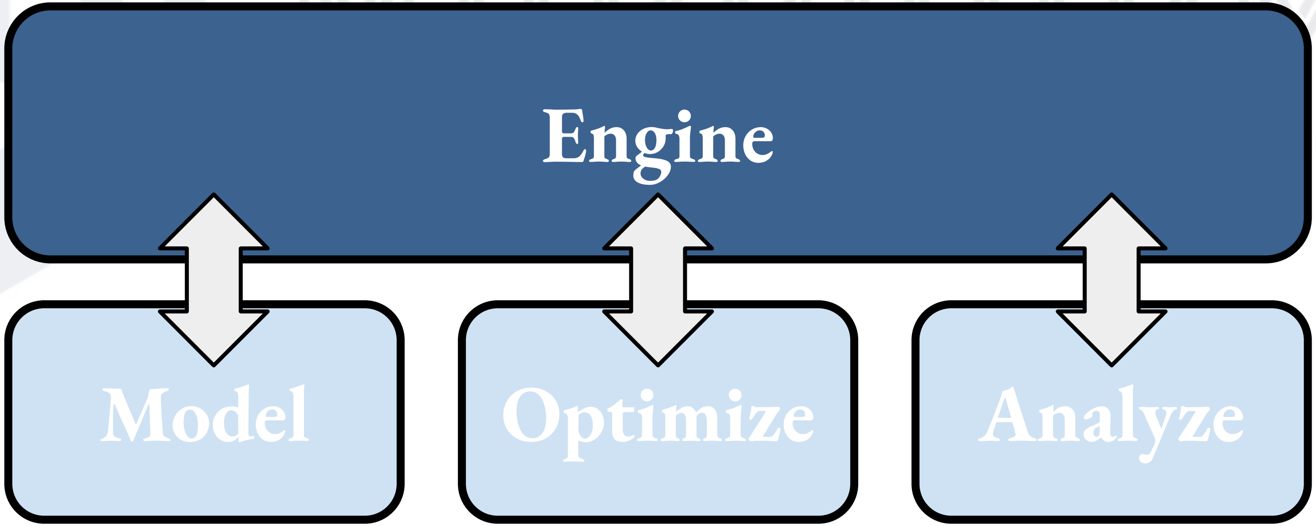






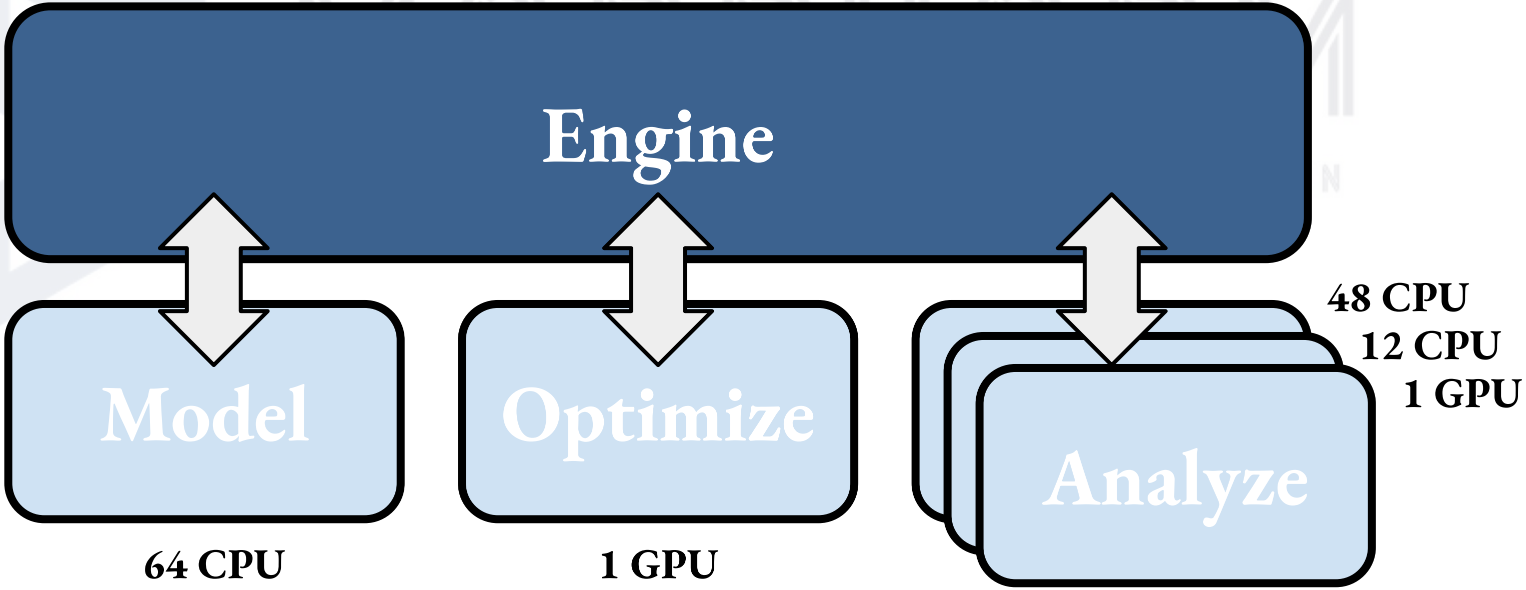


Multiple Program, Multiple Data (MPMD) Engine



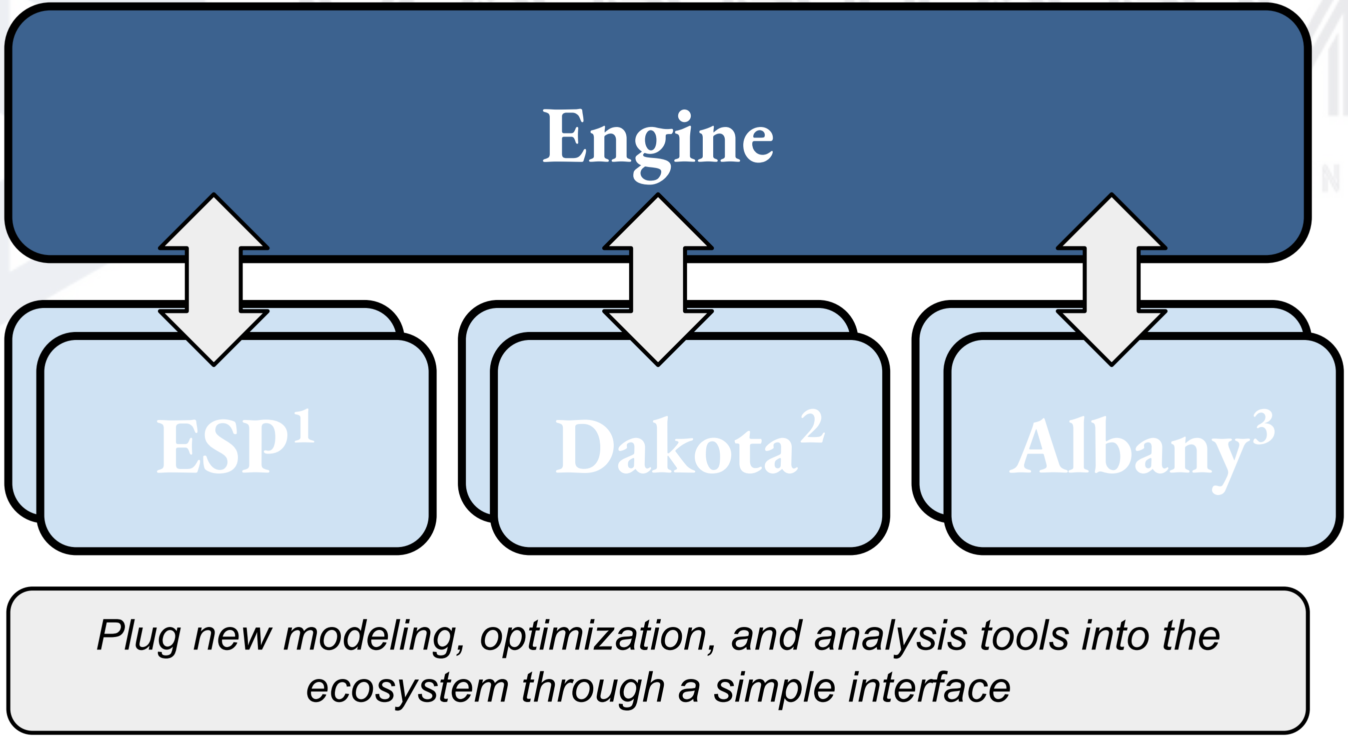
Provides automated management and execution of programs and data transfers at runtime in an HPC environment

MPMD Engine: Concurrent Evaluations



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

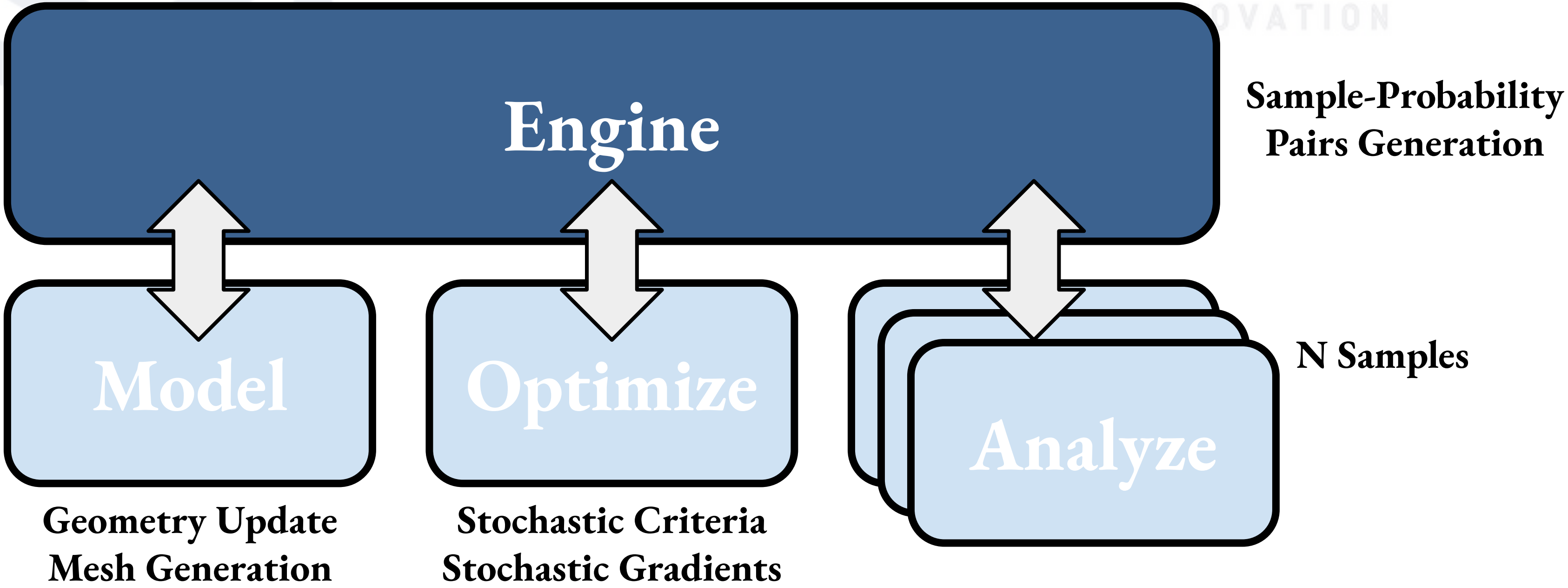
MPMD Engine: Plug-N-Play



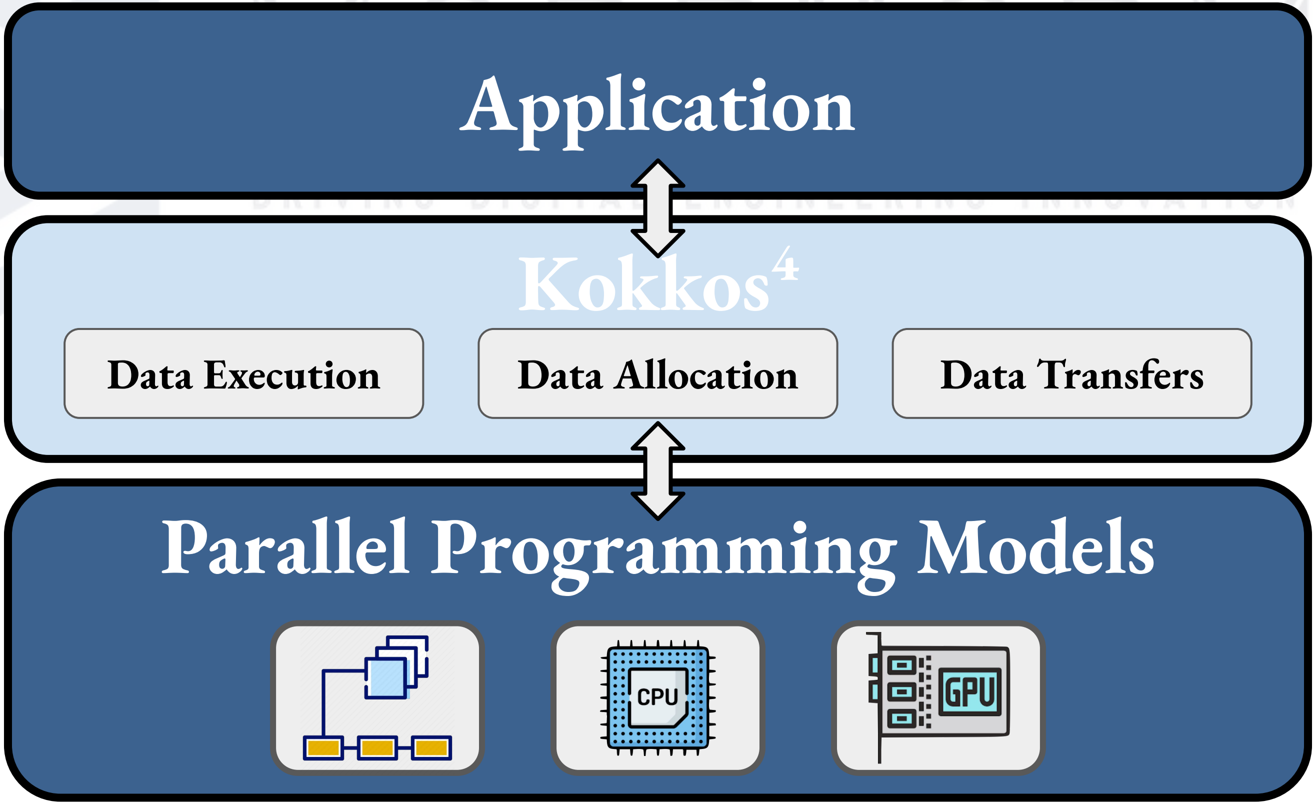
[1] https://acdl.mit.edu/ESP/ (Geometry Modeling Engine) [2] https://dakota.sandia.gov/ (Optimization & UQ Engine) [3] https://github.com/sandialabs/Albany (Multiphysics Simulation Engine)

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/

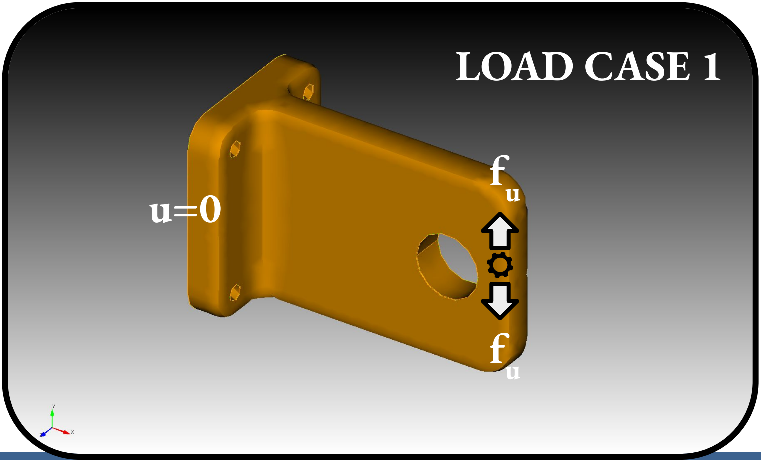
Applications

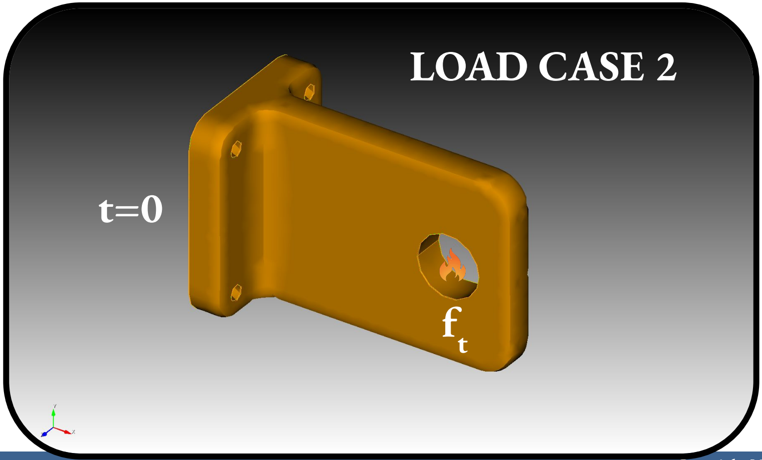
Topology Optimization

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

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

$$\text{with:} \quad \mathbf{K_u}(\mathbf{z})\mathbf{u} = \mathbf{f_u} \quad \text{and} \quad \mathbf{K_t}(\mathbf{z})\mathbf{t} = \mathbf{f_t}$$





Total Derivative

<u>Adjoint Method</u>

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

<u>Adjoint Solve</u>

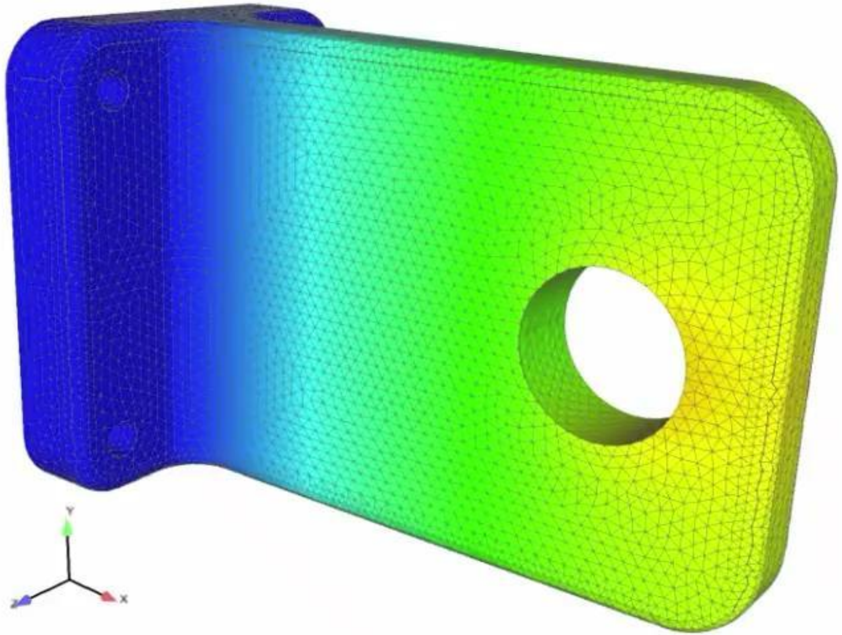
$$\xi = -\left[\left(\frac{\partial \mathbf{R}(\mathbf{z},\mathbf{u})}{\partial \mathbf{u}}\right)^T\right]^{-1} \left(\frac{\partial f(\mathbf{z},\mathbf{u})}{\partial \mathbf{u}}\right)$$

<u>Total Derivative</u>

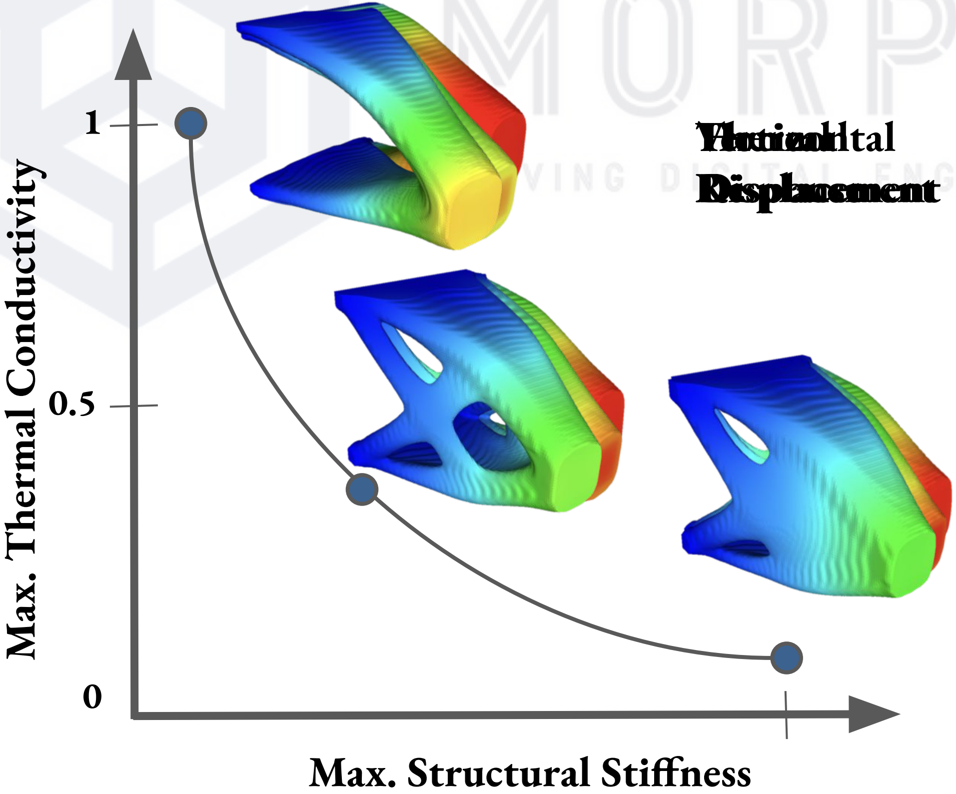
$$\frac{df(\mathbf{z},\mathbf{u})}{d\mathbf{z}} = \frac{\partial f(\mathbf{z},\mathbf{u})}{\partial \mathbf{z}} + \xi^T \frac{\partial \mathbf{R}(\mathbf{z},\mathbf{u})}{\partial \mathbf{z}}$$

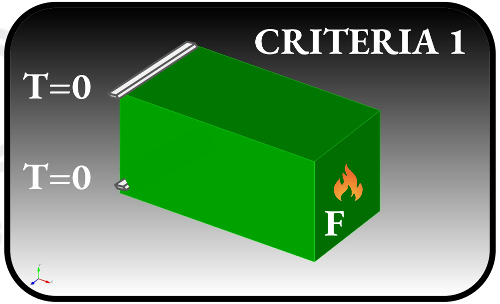
Automatic Differentiation (AD) numerical methods are applied to derive the total derivative!!!

Real-Time Solution

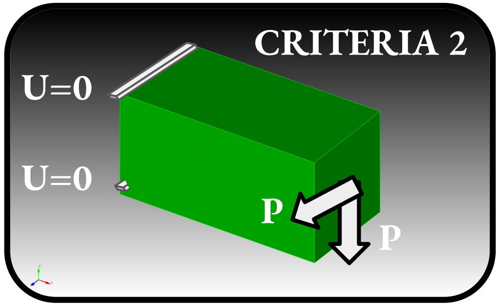


Design Exploration





Max. 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

$$\min_{\mathbf{z}\in[0,1]^N} \quad f(\mathbf{z},\mathbf{u}) = \alpha_1 M(\mathbf{z}) + \alpha_2 \mathbf{f}^T\mathbf{u}$$

$$\text{s.t.} \quad g_j(\mathbf{z},\mathbf{u}) \leq 0 \quad 0,\ldots,j$$

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

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

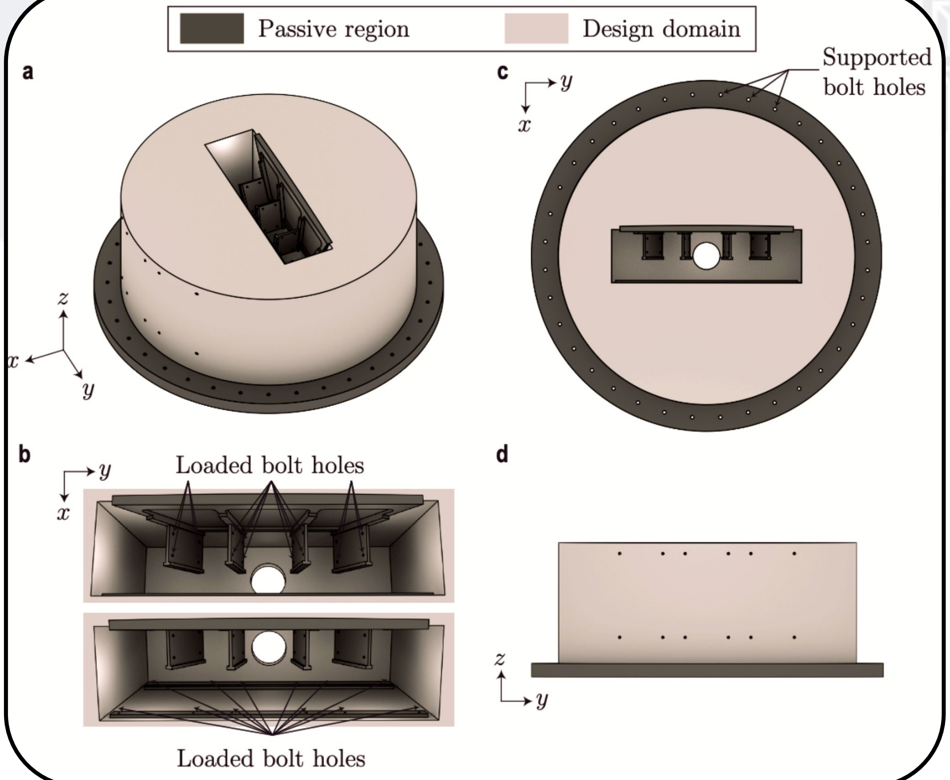
$$\xi^{(k)} = -\left[\left(\frac{\partial \mathbf{R}^{(k)}(\mathbf{z},\mathbf{u})}{\partial \mathbf{u}}\right)^T\right]^{-1} \left(\frac{\partial J^{(k)}(\mathbf{z},\mathbf{u})}{\partial \mathbf{u}}\right)$$

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

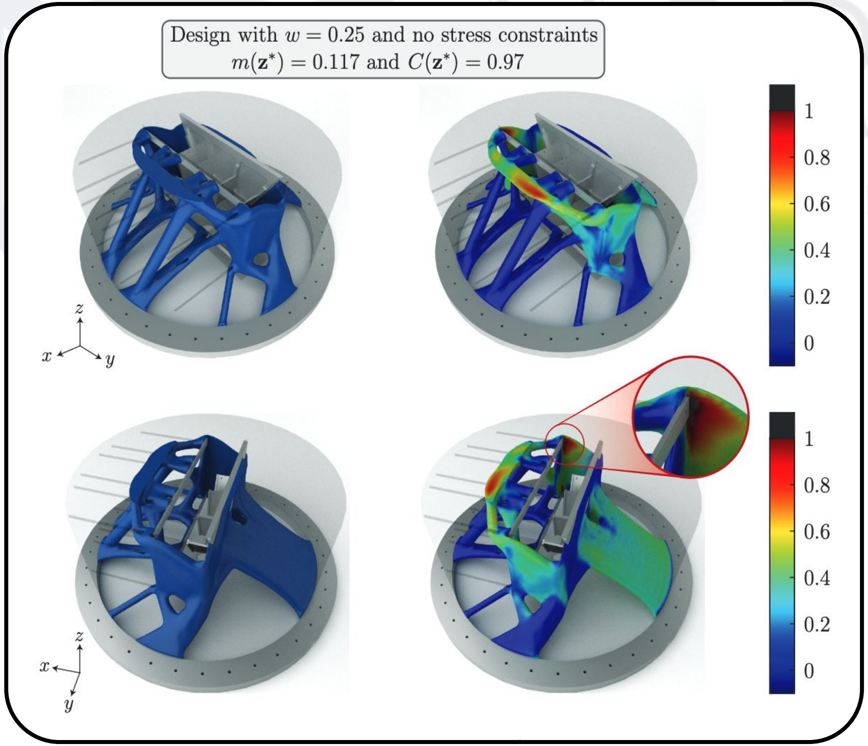
Linear Elasticity

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

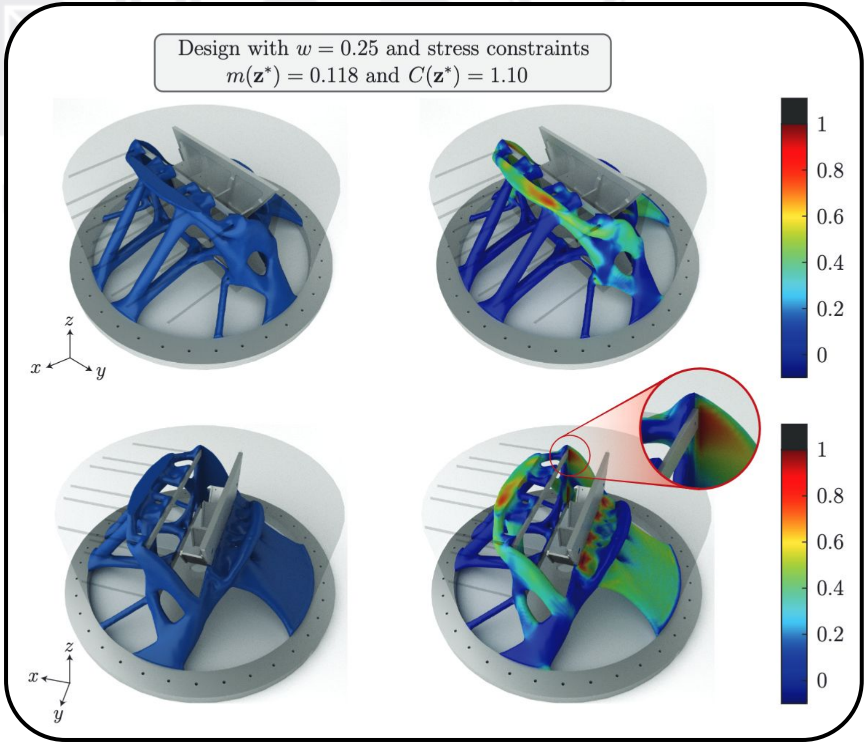
Traction Load: $\{1x10^3, 0.05x10^3, 0.05x10^3\}$

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

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

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

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

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

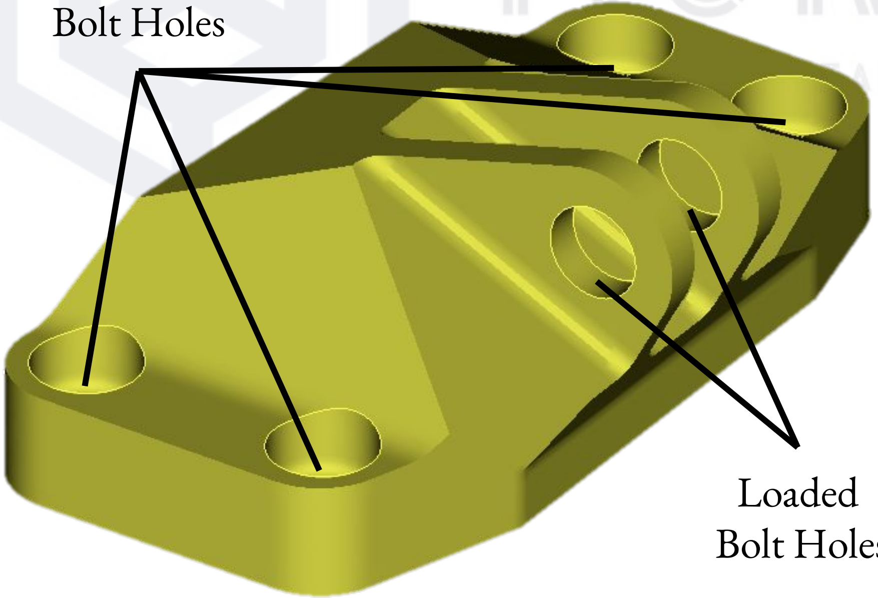
$$\widehat{\mathrm{Std}}\left[\mathbf{C}(\mathbf{z},\mathbf{U};\Theta)\right] = \sqrt{\widehat{\mathbb{E}}\left[\mathbf{C}^2\right] + \widehat{\mathbb{E}}\left[\mathbf{C}\right]^2} = \sqrt{\sum_{j=1}^{M_s}\left(\widehat{\mathbf{c}}^{(j)}\right)^2 p^{(j)} - \left(\sum_{j=1}^{M_s}\widehat{\mathbf{c}}^{(j)}p^{(j)}\right)^2}$$

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: $\mathcal{N}$(70 GPa,10 GPa)
- Poisson's Ratio: 0.33

Traction Load: {$\mathcal{N}$(1 KPa,0.1 KPa), {N(0.5 KPa,0.2 KPa), $\mathcal{N}$(0.5 KPa,0.25 KPa)}

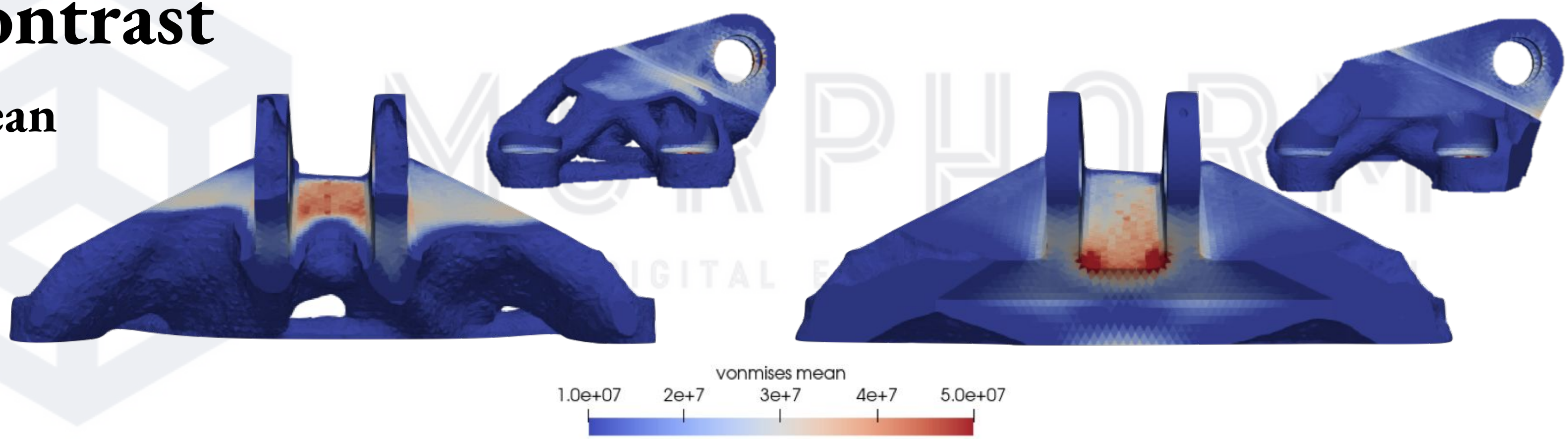
Stress Limit: 140 MPa

Results: Structural Topology Optimization

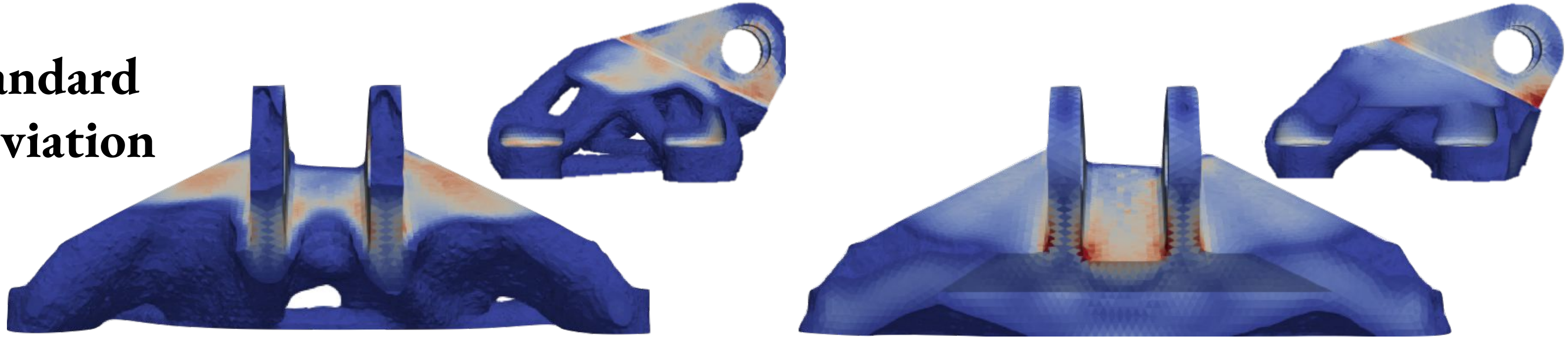
Results: Meet Material Strength Threshold

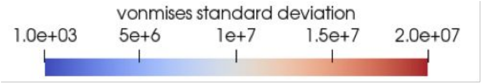
Contrast

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.

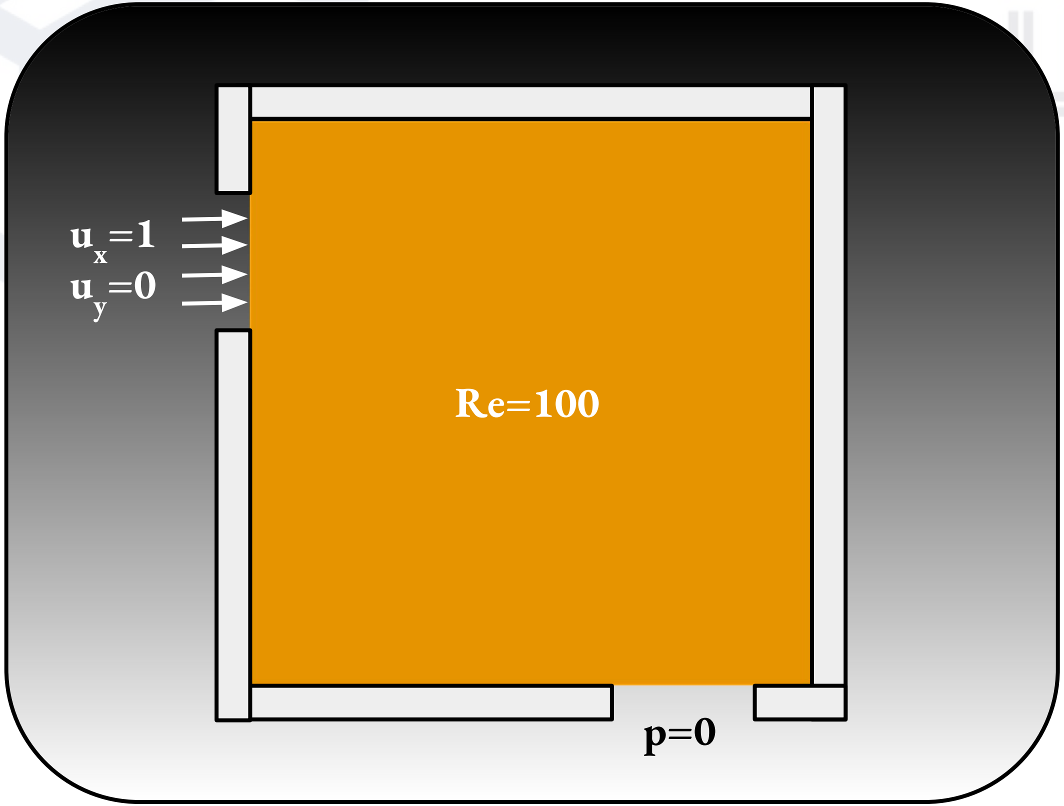
$$
\begin{aligned}
\min_{\mathbf{z}\in[0,1]^N} \quad & \frac{\alpha}{2}\|\mathbf{p}_{in} - \mathbf{p}_{out}\|^2 \\
\text{s.t.} \quad & M(\mathbf{z}) \leq M_{lim} \\
\text{with:} \quad & \frac{\partial \mathbf{u}_i}{\partial \mathbf{x}_i} = 0 \\
& \frac{1}{c^2}\frac{\partial \mathbf{p}}{\partial t} = -\rho_0 \frac{\partial \mathbf{u}_i}{\partial \mathbf{x}_i} \quad \text{in} \quad \Omega \\
& \rho_0\left[\frac{\partial \mathbf{u}_i}{\partial t} + \frac{\partial}{\partial \mathbf{x}_j}\left(\mathbf{u}_i\mathbf{u}_j\right)\right] = -\frac{\partial \mathbf{p}}{\mathbf{x}_i} + \frac{\partial \tau_{ij}}{\partial \mathbf{x}_j} \quad \text{in} \quad \Omega
\end{aligned}
$$

Incompressibility Condition

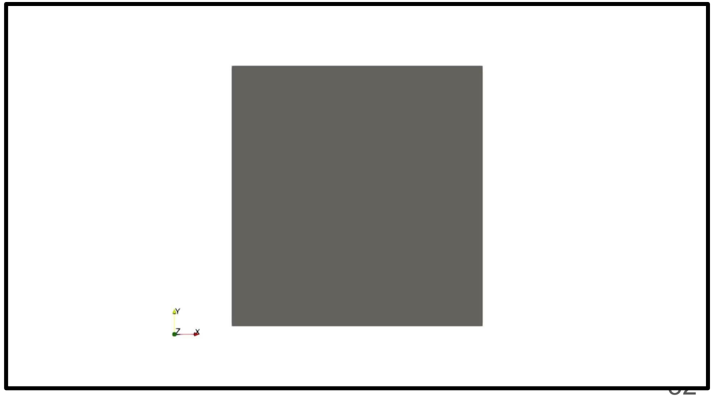
Conservation of Mass

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.

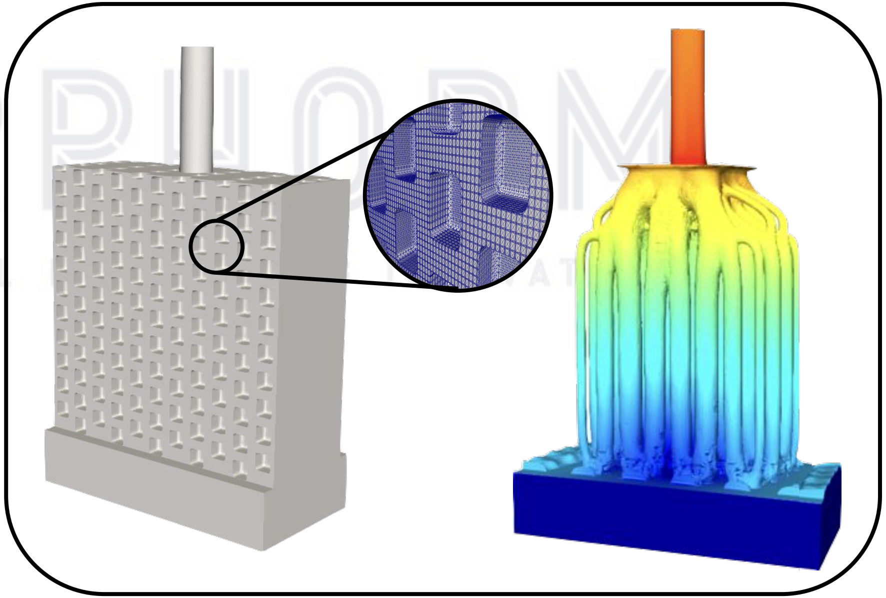


Fluid Velocity Field

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

Thank you for your time

info@morphorm.com

Engineering Desktop