High-order, Time-dependent PDE-Constrained Optimization Using Discontinuous Galerkin Methods (and then some)

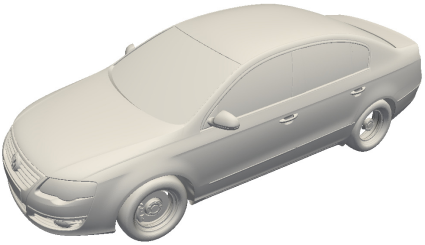
Matthew J. Zahr

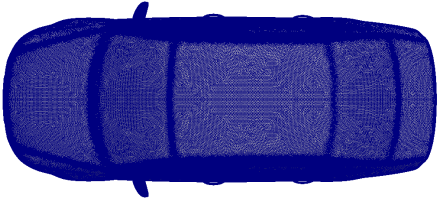
Stanford University
Joint work: Per-Olof Persson (UCB), Charbel Farhat (Stanford U)

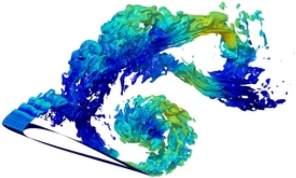
2015 DOE CSGF Annual Program Review
Wednesday, July 29, 2015

Application I: Shape Optimization of Vehicle in Turbulent Flow

- Volkswagen Passat
- Shape optimization
  - Minimum drag configuration
  - Unsteady effects
- Simulation
  - 4M vertices, 24M dof
  - Compressible Navier-Stokes
  - Spalart-Allmaras
- Single forward simulation
  - $\approx$ 1 day on 2048 CPUs

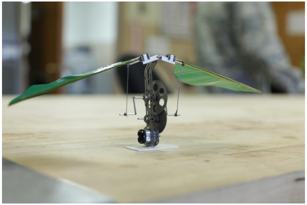




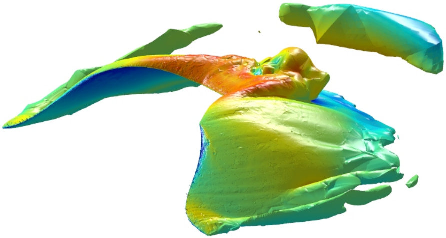


Application II: Optimal Control Flapping Wing

- Biologically-inspired flight
  - Micro Aerial Vehicles (MAVs)
- Mesh
  - 43,000 vertices
  - 231,000 tetra ($p = 3$)
  - 2,310,000 DOF
- CFD
  - Compressible Navier-Stokes
  - Discontinuous Galerkin
- Shape optimization, control
  - unsteady effects
  - min energy, const thrust



Micro Aerial Vehicle

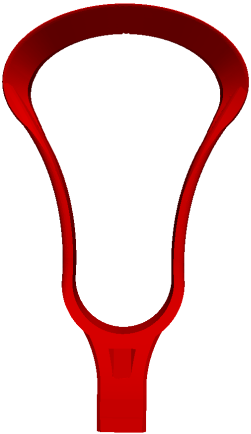


Flapping Wing [Persson et al., 2012]

Application III: Topology Optimization

- Design of new lacrosse head [1]
- Mesh
  - 96,247 vertices
  - 475,666 tetra
  - 276,159 DOF
- Single forward simulation
  - ≈ 5 minutes on 1 core

- Desired: topology optimization
  - Finer mesh (10-100x)
  - Realistic material model

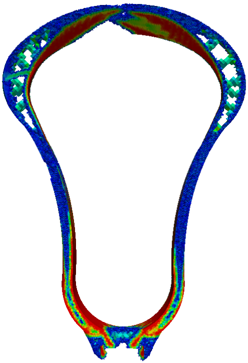


[1] Collaboration with K. Washabaugh

Application III: Topology Optimization

- Design of new lacrosse head [1]
- Mesh
  - 96,247 vertices
  - 475,666 tetra
  - 276,159 DOF
- Single forward simulation
  - $\approx$ 5 minutes on 1 core

- Desired: topology optimization
  - Finer mesh (10-100x)
  - Realistic material model

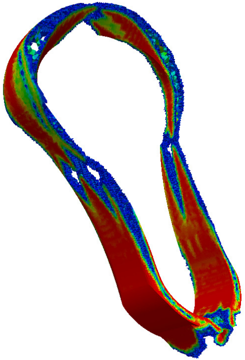


[1] Collaboration with K. Washabaugh

Application III: Topology Optimization

- Design of new lacrosse head [1]
- Mesh
  - 96,247 vertices
  - 475,666 tetra
  - 276,159 DOF
- Single forward simulation
  - $\approx$ 5 minutes on 1 core

- Desired: topology optimization
  - Finer mesh (10-100x)
  - Realistic material model



[1] Collaboration with K. Washabaugh

Problem Formulation

Goal: Find the solution of the *unsteady PDE-constrained optimization* problem

$$\begin{aligned} \underset{\boldsymbol{U},\ \boldsymbol{\mu}}{\text{minimize}} \quad & \mathcal{J}(\boldsymbol{U}, \boldsymbol{\mu}) \\ \text{subject to} \quad & \boldsymbol{C}(\boldsymbol{U}, \boldsymbol{\mu}) \leq 0 \\ & \frac{\partial \boldsymbol{U}}{\partial t} + \nabla \cdot \boldsymbol{F}(\boldsymbol{U}, \nabla \boldsymbol{U}) = 0 \quad \text{in} \quad v(\boldsymbol{\mu}, t) \end{aligned}$$

where

- $\boldsymbol{U}(\boldsymbol{x}, t)$ — PDE solution
- $\boldsymbol{\mu}$ — design/control parameters
- $\mathcal{J}(\boldsymbol{U}, \boldsymbol{\mu}) = \int_{T_0}^{T_f} \int_{\boldsymbol{\Gamma}} j(\boldsymbol{U}, \boldsymbol{\mu}, t)\, dS\, dt$ — objective function
- $\boldsymbol{C}(\boldsymbol{U}, \boldsymbol{\mu}) = \int_{T_0}^{T_f} \int_{\boldsymbol{\Gamma}} \mathbf{c}(\boldsymbol{U}, \boldsymbol{\mu}, t)\, dS\, dt$ — constraints

ALE Description of Conservation Law

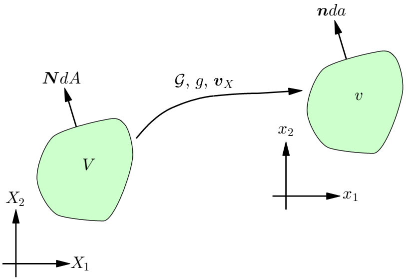
- Map from fixed reference domain V to physical, deformable (parametrized) domain $v(\boldsymbol{\mu}, t)$
- A point $\boldsymbol{X} \in V$ is mapped to $\boldsymbol{x}(\boldsymbol{\mu}, t) = \mathcal{G}(\mathbf{X}, \boldsymbol{\mu}, t) \in v(\boldsymbol{\mu}, t)$

- Introduce transformation

$$\boldsymbol{U}_{\boldsymbol{X}} = g\boldsymbol{U}$$
$$\boldsymbol{F}_{\boldsymbol{X}} = g\boldsymbol{G}^{-1}\boldsymbol{F} - \boldsymbol{U}_{\boldsymbol{X}}\boldsymbol{G}^{-1}\boldsymbol{v}_{\boldsymbol{X}}$$

where

$$\boldsymbol{G} = \nabla_{\boldsymbol{X}}\mathcal{G}, \;\; g = \det \boldsymbol{G}, \;\; \boldsymbol{v}_{\boldsymbol{X}} = \left.\frac{\partial \mathcal{G}}{\partial t}\right|_{\boldsymbol{X}}$$



- Transformed conservation law

$$\left.\frac{\partial \boldsymbol{U}_{\boldsymbol{X}}}{\partial t}\right|_{\boldsymbol{X}} + \nabla_{\boldsymbol{X}} \cdot \boldsymbol{F}_{\boldsymbol{X}}(\boldsymbol{U}_{\boldsymbol{X}}, \; \nabla_{\boldsymbol{X}}\boldsymbol{U}_{\boldsymbol{X}}) = 0$$

Spatial Discretization: Discontinuous Galerkin

- Re-write conservation law as first-order system

$$\left.\frac{\partial \boldsymbol{U_X}}{\partial t}\right|_{\boldsymbol{X}} + \nabla_{\boldsymbol{X}} \cdot \boldsymbol{F_X}(\boldsymbol{U_X},\ \boldsymbol{Q_X}) = 0$$

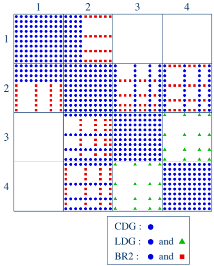
$$\boldsymbol{Q_X} - \nabla_{\boldsymbol{X}} \boldsymbol{U_X} = 0$$

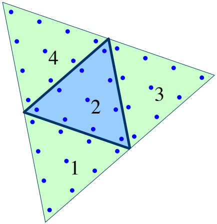
- Discretize using DG

- Roe's method for inviscid flux
- Compact DG (CDG) for viscous flux
- *Semi-discrete* equations

$$\mathbb{M}\frac{\partial \boldsymbol{u}}{\partial t} = \boldsymbol{r}(\boldsymbol{u}, \boldsymbol{\mu}, t)$$

$$\boldsymbol{u}(0) = \boldsymbol{u}_0(\boldsymbol{\mu})$$





Stencil for CDG, LDG, and BR2 fluxes

Temporal Discretization: Diagonally-Implicit Runge-Kutta

- Diagonally-Implicit RK (DIRK) are implicit Runge-Kutta schemes defined by lower triangular Butcher tableau $\rightarrow$ **decoupled implicit stages**
- Overcomes issues with high-order BDF and IRK
    - Limited accuracy of A-stable BDF schemes (2nd order)
    - High cost of general implicit RK schemes (coupled stages)

$$\boldsymbol{u}^{(0)} = \boldsymbol{u}_0(\boldsymbol{\mu})$$

$$\boldsymbol{u}^{(n)} = \boldsymbol{u}^{(n-1)} + \sum_{i=1}^{s} b_i \boldsymbol{k}_i^{(n)}$$

$$\boldsymbol{u}_i^{(n)} = \boldsymbol{u}^{(n-1)} + \sum_{j=1}^{i} a_{ij} \boldsymbol{k}_j^{(n)}$$

$$\mathbb{M}\boldsymbol{k}_i^{(n)} = \Delta t_n \boldsymbol{r}\left(\boldsymbol{u}_i^{(n)},\ \boldsymbol{\mu},\ t_{n-1} + c_i \Delta t_n\right)$$

$$\begin{array}{c|cccc}
c_1 & a_{11} & & & \\
c_2 & a_{21} & a_{22} & & \\
\vdots & \vdots & \vdots & \ddots & \\
c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\
\hline
 & b_1 & b_2 & \cdots & b_s
\end{array}$$

Butcher Tableau for DIRK scheme

Fully-Discrete Adjoint Equations

$$\boldsymbol{\lambda}^{(N_t)} = \frac{\partial F}{\partial \boldsymbol{u}^{(N_t)}}^T$$

$$\boldsymbol{\lambda}^{(n-1)} = \boldsymbol{\lambda}^{(n)} + \frac{\partial F}{\partial \boldsymbol{u}^{(n-1)}}^T + \sum_{i=1}^{s} \Delta t_n \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{u}} \left(\boldsymbol{u}_i^{(n)},\ \boldsymbol{\mu},\ t_{n-1} + c_i \Delta t_n\right)^T \boldsymbol{\kappa}_i^{(n)}$$

$$\mathbb{M}^T \boldsymbol{\kappa}_i^{(n)} = \sum_{j=i}^{s} a_{ji} \Delta t_n \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{u}} \left(\boldsymbol{u}_j^{(n)},\ \boldsymbol{\mu},\ t_{n-1} + c_j \Delta t_n\right)^T \boldsymbol{\kappa}_j^{(n)}$$

- **Linear** evolution equations solved **backward** in time
  - Requires solving linear systems of equations with $\frac{\partial \boldsymbol{r}}{\partial \boldsymbol{u}}^T$
  - Accurate solution of linear system required
- Primal state, $\boldsymbol{u}^{(n)}$, and stage, $\boldsymbol{k}_i^{(n)}$, required at each state/stage of dual solve
  - Parallel I/O
- Heavily-dependent on **chosen ouput**
  - $\boldsymbol{\lambda}^{(n)}$ and $\boldsymbol{\kappa}_i^{(n)}$ must be computed for each output functional F

Gradient Reconstruction via Dual Variables

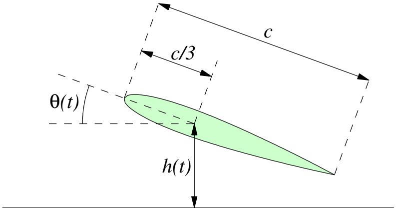
- Equipped with the solution to the primal problem, $\boldsymbol{u}^{(n)}$ and $\boldsymbol{k}_i^{(n)}$, and dual problem, $\boldsymbol{\lambda}^{(n)}$ and $\boldsymbol{\kappa}_i^{(n)}$, the output gradient is reconstructed as

$$\frac{\mathrm{d}F}{\mathrm{d}\boldsymbol{\mu}} = \frac{\partial F}{\partial \boldsymbol{\mu}} - \boldsymbol{\lambda}^{(0)\,T}\frac{\partial \boldsymbol{u}_0}{\partial \boldsymbol{\mu}} - \sum_{n=1}^{N_t} \Delta t_n \sum_{i=1}^{s} \boldsymbol{\kappa}_i^{(n)\,T} \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{\mu}}(\boldsymbol{u}_i^{(n)},\ \boldsymbol{\mu},\ t_i^{(n)})$$

- Independent of sensitivities, $\dfrac{\partial \boldsymbol{u}^{(n)}}{\partial \boldsymbol{\mu}}$ and $\dfrac{\partial \boldsymbol{k}_i^{(n)}}{\partial \boldsymbol{\mu}}$

Problem Setup

$$\begin{aligned}
\underset{h(t),\theta(t)}{\text{maximize}} \quad & \int_0^T \int_{\boldsymbol{\Gamma}} \boldsymbol{f} \cdot \boldsymbol{v} \, dS \, dt \\
\text{subject to} \quad & h(0) = h'(0) = h'(T) = 0, \;\; h(T) = 1 \\
& \theta(0) = \theta'(0) = \theta(T) = \theta'(T) = 0 \\
& \frac{\partial \boldsymbol{U}}{\partial t} + \nabla \cdot \boldsymbol{F}(\boldsymbol{U}, \nabla \boldsymbol{U}) = 0
\end{aligned}$$



Airfoil schematic, kinematic description

- Non-zero freestream velocity
- $h(t)$, $\theta(t)$ discretized via *clamped cubic splines*
- Knots of cubic splines as optimization parameters, $\boldsymbol{\mu}$
- Black-box optimizer: SNOPT

Optimization Results: Vorticity Field History

Energy $= -1.47$	Energy $= -0.120$	Energy $= 0.756$
$h_0(t),\ \theta_0(t)$	$h_0(t),\ \theta^*(t)$	$h^*(t),\ \theta^*(t)$

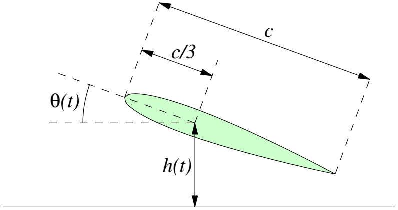
$\boxed{\text{Play/Pause}}$

Initial Guess: $h_0(t),\ \theta_0(t)$

Problem Setup

$$\begin{aligned} \underset{h(t),\theta(t)}{\text{maximize}} \quad & \int_0^T \int_{\boldsymbol{\Gamma}} \boldsymbol{f} \cdot \boldsymbol{v} \, dS \, dt \\ \text{subject to} \quad & -\int_0^T \int_{\boldsymbol{\Gamma}} F_x \, dS \, dt \geq c \\ & h^{(k)}(t) = h^{(k)}(t+T) \\ & \theta^{(k)}(t) = \theta^{(k)}(t+T) \\ & \frac{\partial \boldsymbol{U}}{\partial t} + \nabla \cdot \boldsymbol{F}(\boldsymbol{U}, \nabla \boldsymbol{U}) = 0 \end{aligned}$$

- Non-zero freestream velocity
- $h(t)$, $\theta(t)$ discretized via phase/amplitude of *Fourier modes*
- Knots of cubic splines as optimization parameters, $\boldsymbol{\mu}$
- Black-box optimizer: SNOPT



Airfoil schematic, kinematic description

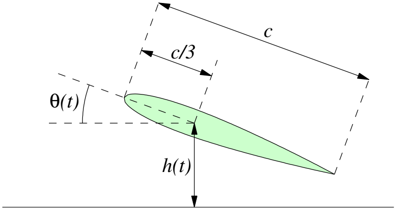
Optimization Results: Vorticity Field History

Energy = -9.51 Thrust = 0.198	Energy = -0.455 Thrust = 0.0	Energy = -1.61 Thrust = 0.7
$h_0(t)$, $\theta_0(t)$	$h^*(t)$, $\theta^*(t)$	$h^{**}(t)$, $\theta^{**}(t)$

Play/Pause

Problem Setup

$$\begin{aligned} \underset{\boldsymbol{w}}{\text{maximize}} \quad & \int_0^T \int_{\boldsymbol{\Gamma}} \boldsymbol{f} \cdot \boldsymbol{v} \, dS \, dt \\ \text{subject to} \quad & \frac{\partial \boldsymbol{U}}{\partial t} + \nabla \cdot \boldsymbol{F}(\boldsymbol{U}, \nabla \boldsymbol{U}) = 0 \end{aligned}$$

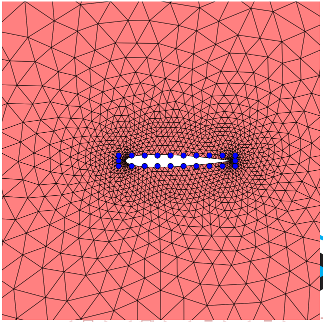


Airfoil schematic, kinematic description

- Radial basis function parametrization

$$\boldsymbol{X}' = \boldsymbol{X} + \boldsymbol{v} + \sum \boldsymbol{w}_i \Phi(||\boldsymbol{X} - \boldsymbol{c}_i||)$$

- *Zero* freestream velocity
- $h(t)$, $\theta(t)$ *prescribed*
- Black-box optimizer: SNOPT



Optimization Results: Vorticity Field History

Energy = -1.01

Energy = -0.609

Initial

Optimal

Play/Pause

Reduced-Order Model

- Model Order Reduction (MOR) assumption: *state vector lies in low-dimensional affine subspace*

$$\boldsymbol{u} \approx \boldsymbol{\Phi} \boldsymbol{y} \qquad \Longrightarrow \qquad \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{\mu}} \approx \frac{\partial \boldsymbol{u}_r}{\partial \boldsymbol{\mu}} = \boldsymbol{\Phi} \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{\mu}}$$

  where $\boldsymbol{y} \in \mathbb{R}^n$ are the reduced coordinates of $\boldsymbol{u}_r$ in the basis $\boldsymbol{\Phi} \in \mathbb{R}^{N \times n}$, and $n \ll N$

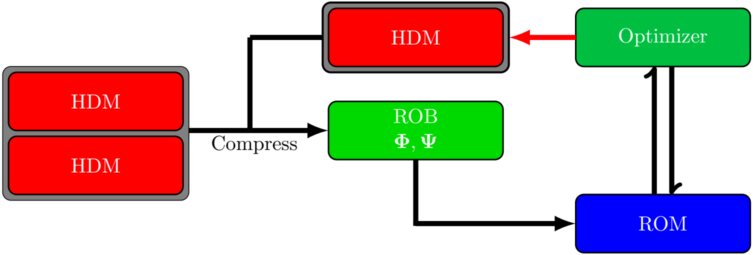
- Substitute assumption into High-Dimensional Model (HDM), $\boldsymbol{R}(\boldsymbol{u}, \boldsymbol{\mu}) = 0$

$$\boldsymbol{R}(\boldsymbol{\Phi} \boldsymbol{y}, \boldsymbol{\mu}) \approx 0$$

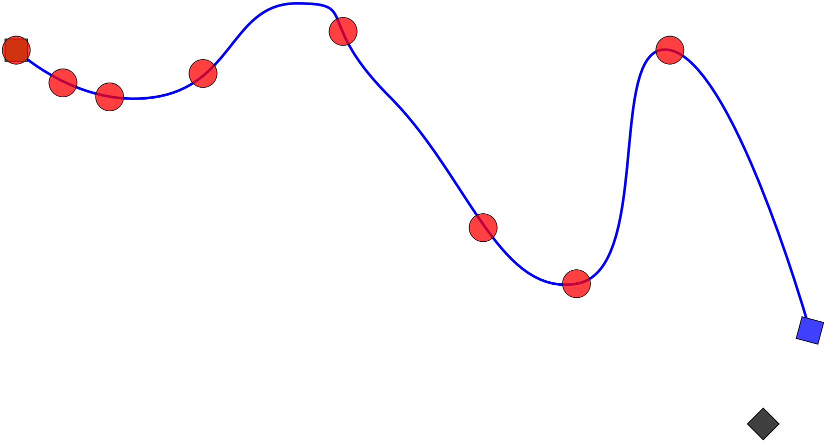
- Require projection of residual in low-dimensional *left subspace*, with basis $\boldsymbol{\Psi} \in \mathbb{R}^{N \times n}$ to be zero

$$\boxed{\boldsymbol{R}_r(\boldsymbol{y}, \boldsymbol{\mu}) = \boldsymbol{\Psi}^T \boldsymbol{R}(\boldsymbol{\Phi} \boldsymbol{y}, \boldsymbol{\mu}) = 0}$$

Adaptive Approach to ROM-Constrained Optimization



Adaptive Approach to ROM-Constrained Optimization



Adaptive Approach to ROM-Constrained Optimization

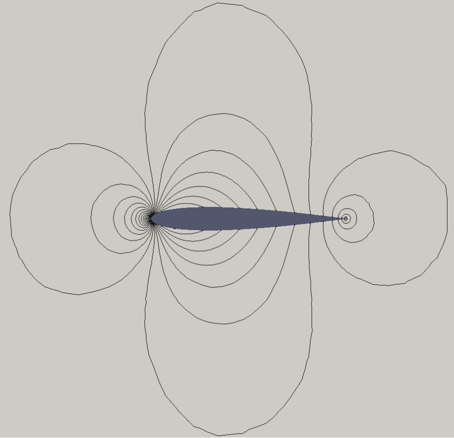
Adaptive Approach to ROM-Constrained Optimization

- Collect snapshots from HDM at *sparse sampling* of the parameter space
  - Initial condition for optimization problem
- Build ROB $\mathbf{\Phi}$ from sparse training
- Solve optimization problem

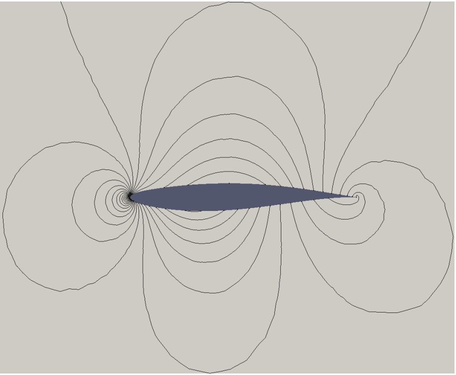
$$\begin{aligned} \underset{\boldsymbol{y}\in\mathbb{R}^n,\ \boldsymbol{\mu}\in\mathbb{R}^p}{\text{minimize}} \quad & f(\mathbf{\Phi}\boldsymbol{y},\boldsymbol{\mu}) \\ \text{subject to} \quad & \mathbf{\Psi}^T\boldsymbol{R}(\mathbf{\Phi}\boldsymbol{y},\boldsymbol{\mu}) = 0 \\ & \frac{1}{2}||\boldsymbol{R}(\mathbf{\Phi}\boldsymbol{y},\boldsymbol{\mu})||_2^2 \leq \epsilon \end{aligned}$$

- Use solution of above problem to enrich training and repeat until convergence

Compressible, Inviscid Airfoil Inverse Design



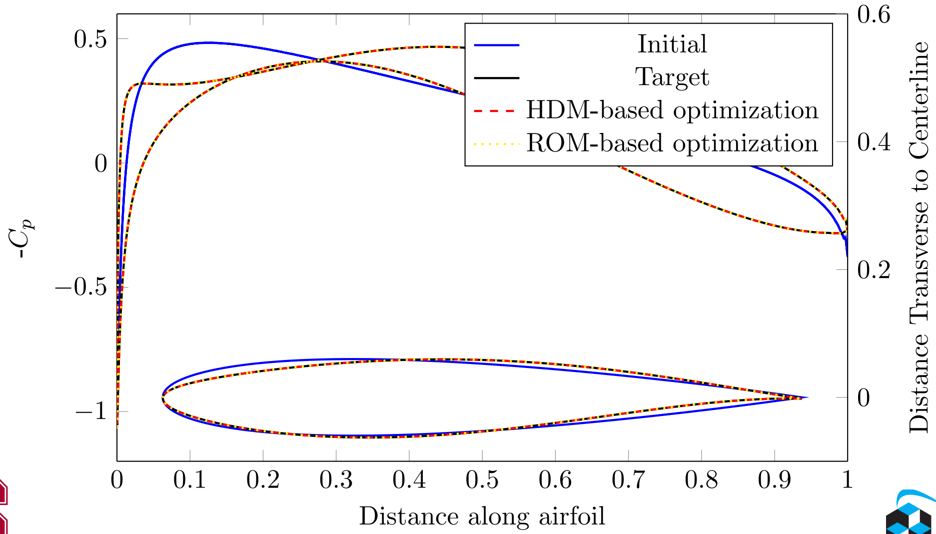
(a) NACA0012: Pressure field ($M_\infty = 0.5$, $\alpha = 0.0°$)



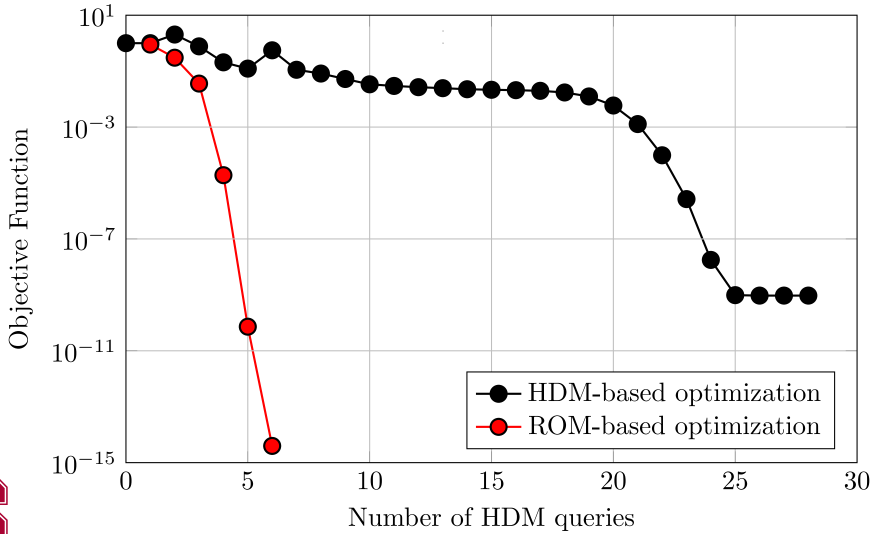
(b) RAE2822: Pressure field ($M_\infty = 0.5$, $\alpha = 0.0°$)

- Pressure discrepancy minimization (Euler equations)
  - Initial Configuration: NACA0012
  - Target Configuration: RAE2822

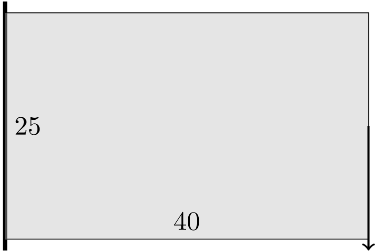
Optimization Results



Optimization Results



Problem Setup

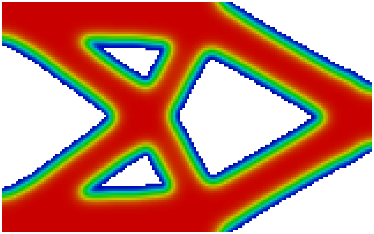


- 16000 8-node brick elements, 77760 dofs
- Total Lagrangian form, finite strain, StVK
- St. Venant-Kirchhoff material
- Sparse Cholesky linear solver (CHOLMOD)
- Newton-Raphson nonlinear solver
- Minimum compliance optimization problem

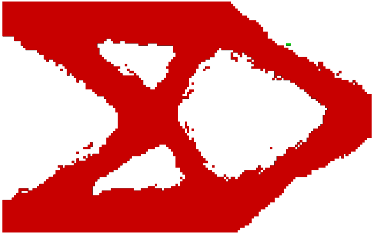
$$\begin{aligned} \underset{\mathbf{u}\in\mathbb{R}^{n_{\mathbf{u}}},\ \boldsymbol{\mu}\in\mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad & \mathbf{f}_{\text{ext}}{}^{T}\mathbf{u} \\ \text{subject to} \quad & V(\boldsymbol{\mu}) \leq \frac{1}{2}V_0 \\ & \mathbf{r}(\mathbf{u},\ \boldsymbol{\mu}) = 0 \end{aligned}$$

- Gradient computations: Adjoint method
- Optimizer: SNOPT
- Maximum ROM size: $k_{\mathbf{u}} \leq 5$

Optimal Solution Comparison



HDM



CTRPOD + Φ_μ adaptivity

HDM Solution	**HDM** Gradient	**HDM** Optimization
7458s (450)	4018s (411)	8284s

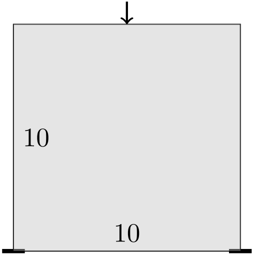
HDM
Elapsed time = 19761s

HDM Solution	**HDM** Gradient	**ROB** Construction	**ROM** Optimization
1049s (64)	88s (9)	727s (56)	39s (3676)

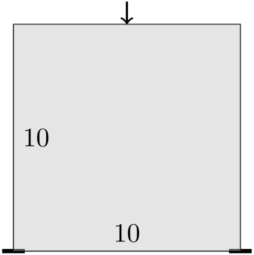
CTRPOD + Φ_μ adaptivity
Elapsed time = 2197s, Speedup ≈ 9x

CTRPOD + Φ_μ adaptivity

Problem Setup



(a) XY view



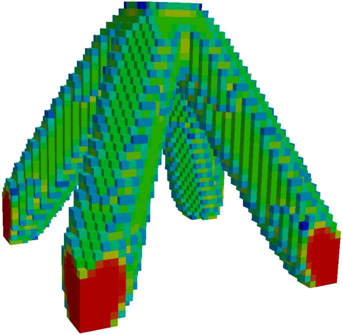
(b) XZ view

- 64000 8-node brick elements, 206715 dofs
- Total Lagrangian formulation, finite strain
- St. Venant-Kirchhoff material
- Jacobi-Preconditioned Conjugate Gradient
- Newton-Raphson nonlinear solver
- Minimum compliance optimization problem

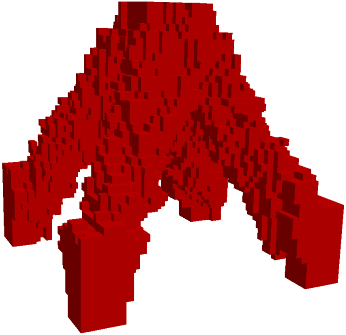
$$\begin{aligned} \underset{\mathbf{u}\in\mathbb{R}^{n_\mathbf{u}},\ \boldsymbol{\mu}\in\mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad & \mathbf{f}_{\text{ext}}{}^T\mathbf{u} \\ \text{subject to} \quad & V(\boldsymbol{\mu}) \leq 0.15 \cdot V_0 \\ & \mathbf{r}(\mathbf{u},\ \boldsymbol{\mu}) = 0 \end{aligned}$$

- Gradient computations: Adjoint method
- Optimizer: SNOPT
- Maximum ROM size: $k_{\mathbf{u}} \leq 5$

Optimal Solution Comparison



HDM

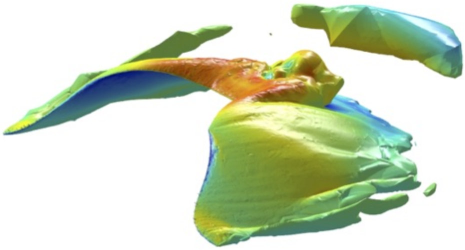


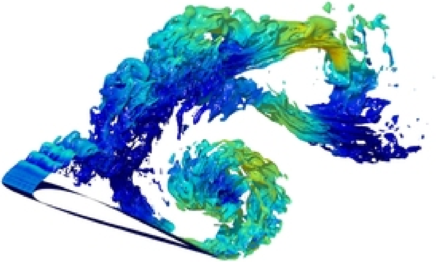
CTRPOD + Φ_μ adaptivity

- **HDM**, elapsed time = 179176s
- **CTRPOD**+Φ_μ adaptivity, elapsed time = 15208s
- Speedup $\approx 12\times$

Future Work

- Application of the method to real-world **3D problems**
- Extension of the method to **multiphysics** problems, such as FSI
- Extension of the method to **chaotic** problems, such as LES flows, where care must be taken to ensure the sensitivities are well-defined
- Incorporation of **adaptive model reduction** technology to further reduce the cost of unsteady optimization





Thank You!

DOE
CSGF

References I

Arian, E., Fahl, M., and Sachs, E. W. (2000).
Trust-region proper orthogonal decomposition for flow control.
Technical report, DTIC Document.

Persson, P.-O., Willis, D., and Peraire, J. (2012).
Numerical simulation of flapping wings using a panel method and a high-order navier–stokes solver.
International Journal for Numerical Methods in Engineering, 89(10):1296–1316.

Zahr, M. J. and Farhat, C. (2014).
Progressive construction of a parametric reduced-order model for pde-constrained optimization.
International Journal for Numerical Methods in Engineering.