An acceleration framework for parameter estimation using implicit sampling and adaptive reduced-order models

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MS91: Large-scale PDE-constrained optimization algorithms and applications
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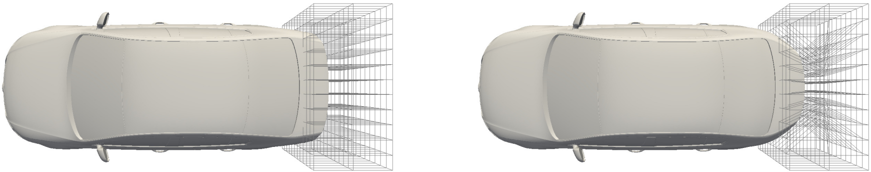
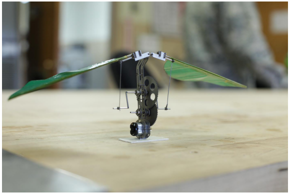
University of Notre Dame

PDE optimization is ubiquitous in science and engineering

Design: Find system that optimizes performance metric, satisfies constraints



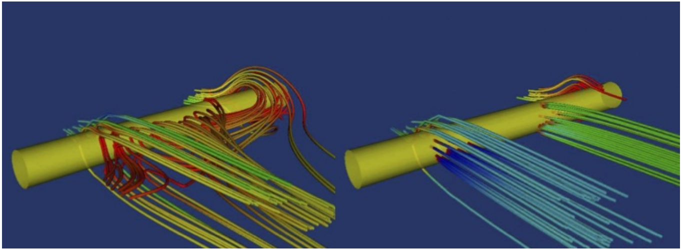
Aerodynamic shape design of automobile



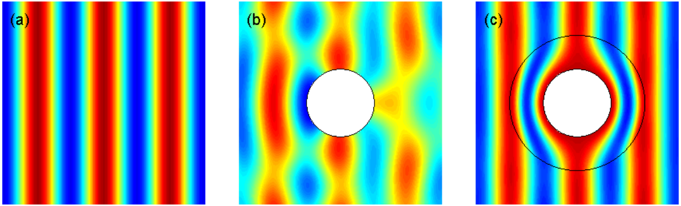
Optimal flapping motion of micro aerial vehicle

PDE optimization is ubiquitous in science and engineering

Control: Drive system to a desired state



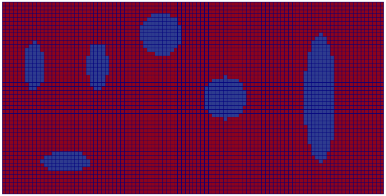
Boundary flow control

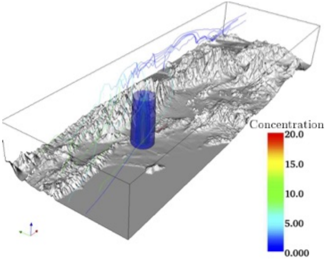


Metamaterial cloaking – electromagnetic invisibility

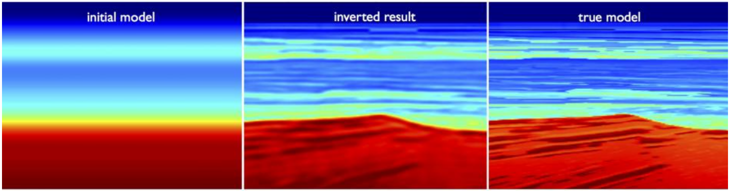
PDE optimization is ubiquitous in science and engineering

Inverse problems: Infer the problem setup given solution observations





Left: Material inversion: find defects from acoustic, structural measurements
Right: Source inversion: find source of airborne contaminant from measurements



Full waveform inversion: estimate subsurface from acoustic measurements

Deterministic[1] PDE-constrained optimization formulation

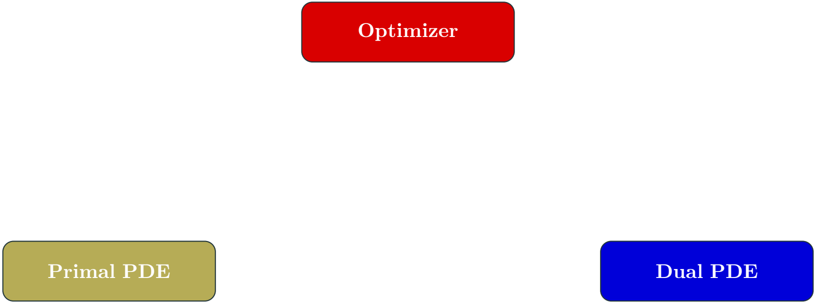
$$\begin{aligned} \underset{\boldsymbol{\mu}\in\mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad & \mathcal{J}(\boldsymbol{u},\, \boldsymbol{\mu}) \\ \text{subject to} \quad & \boldsymbol{r}(\boldsymbol{u},\, \boldsymbol{\mu}) = 0 \end{aligned}$$

$\boldsymbol{r} : \mathbb{R}^{n_{\boldsymbol{u}}} \times \mathbb{R}^{n_{\boldsymbol{\mu}}} \to \mathbb{R}^{n_{\boldsymbol{u}}}$	discretized PDE
$\mathcal{J} : \mathbb{R}^{n_{\boldsymbol{u}}} \times \mathbb{R}^{n_{\boldsymbol{\mu}}} \to \mathbb{R}$	quantity of interest
$\boldsymbol{u} \in \mathbb{R}^{n_{\boldsymbol{u}}}$	PDE state vector
$\boldsymbol{\mu} \in \mathbb{R}^{n_{\boldsymbol{\mu}}}$	optimization parameters

[1] Extension to stochastic see MS280 on Thursday

Nested approach to PDE-constrained optimization

Virtually all expense emanates from primal/dual PDE solves



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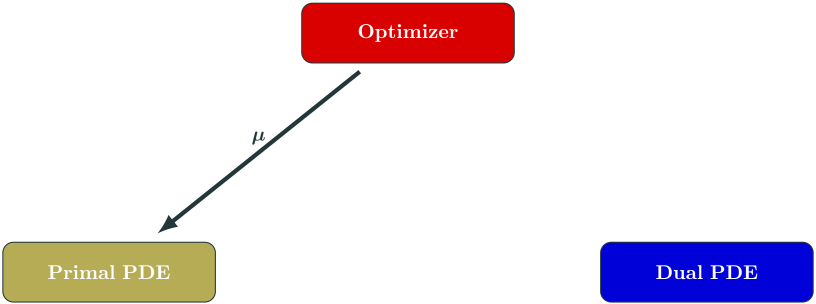

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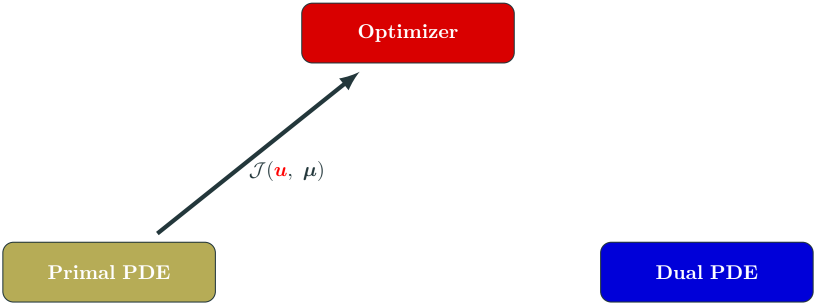

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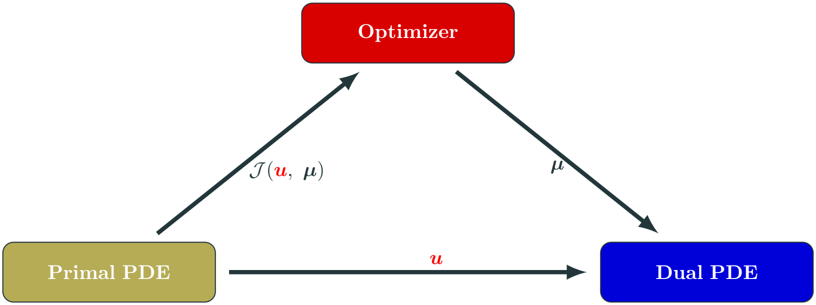

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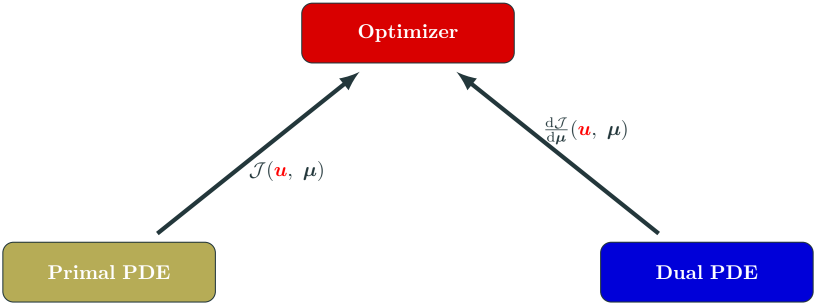

Efficient PDE-constrained optimization using managed inexactness

Application to Bayesian parameter estimation

Efficient PDE-constrained optimization using managed inexactness

Proposed approach: managed inexactness

Replace expensive PDE with inexpensive approximation model

- **Reduced-order models** used for *inexact PDE evaluations*
- **Partially converged solutions** used for *inexact PDE evaluations*

$$\underset{\boldsymbol{\mu} \in \mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad F(\boldsymbol{\mu}) \qquad \longrightarrow \qquad \underset{\boldsymbol{\mu} \in \mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad m(\boldsymbol{\mu})$$

[2] Must be *computable* and apply to general, nonlinear PDEs

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Manage inexactness with trust region method

- Embedded in globally convergent **trust region** method
- **Error indicators**[2] to account for *all* sources of inexactness
- **Refinement** of approximation model using *greedy algorithms*

$$\underset{\boldsymbol{\mu}\in\mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} \quad F(\boldsymbol{\mu}) \qquad \longrightarrow \qquad \begin{array}{ll} \underset{\boldsymbol{\mu}\in\mathbb{R}^{n_{\boldsymbol{\mu}}}}{\text{minimize}} & m_k(\boldsymbol{\mu}) \\ \text{subject to} & ||\boldsymbol{\mu} - \boldsymbol{\mu}_k|| \leq \Delta_k \end{array}$$

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Relationship between the objective function and model

- First-order consistency [Alexandrov et al., 1998]

$$m_k(\boldsymbol{\mu}_k) = F(\boldsymbol{\mu}_k) \qquad \nabla m_k(\boldsymbol{\mu}_k) = \nabla F(\boldsymbol{\mu}_k)$$

- The Carter condition [Carter, 1989, Carter, 1991]

$$||\nabla F(\boldsymbol{\mu}_k) - \nabla m_k(\boldsymbol{\mu}_k)|| \leq \eta \, ||\nabla m_k(\boldsymbol{\mu}_k)|| \qquad \eta \in (0,\, 1)$$

- Asymptotic gradient bound [Heinkenschloss and Vicente, 2002]

$$||\nabla F(\boldsymbol{\mu}_k) - \nabla m_k(\boldsymbol{\mu}_k)|| \leq \xi \min\{||\nabla m_k(\boldsymbol{\mu}_k)|| \,,\, \Delta_k\} \qquad \xi > 0$$

Asymptotic gradient bound permits the use of an ***error indicator****:* φ_k

$$||\nabla F(\boldsymbol{\mu}) - \nabla m_k(\boldsymbol{\mu})|| \leq \xi \varphi_k(\boldsymbol{\mu}) \qquad \xi > 0$$
$$\varphi_k(\boldsymbol{\mu}_k) \leq \kappa_\varphi \min\{||\nabla m_k(\boldsymbol{\mu}_k)|| \,,\, \Delta_k\}$$

Trust region method with inexact gradients [Kouri et al., 2013]

1: **Model update**: Choose model m_k such that error indicator φ_k satisfies

$$\varphi_k(\boldsymbol{\mu}_k) \leq \kappa_\varphi \min\{||\nabla m_k(\boldsymbol{\mu}_k)||\,,\, \Delta_k\}$$

2: **Step computation**: Approximately solve the trust region subproblem

$$\hat{\boldsymbol{\mu}}_k \quad = \quad \underset{\boldsymbol{\mu}\in\mathbb{R}^{n_{\boldsymbol{\mu}}}}{\arg\min}\; m_k(\boldsymbol{\mu}) \quad \text{subject to} \quad ||\boldsymbol{\mu} - \boldsymbol{\mu}_k|| \leq \Delta_k$$

3: **Step acceptance**: Compute actual-to-predicted reduction

$$\rho_k = \frac{F(\boldsymbol{\mu}_k) - F(\hat{\boldsymbol{\mu}}_k)}{m_k(\boldsymbol{\mu}_k) - m_k(\hat{\boldsymbol{\mu}}_k)}$$

if $\rho_k \geq \eta_1$ **then** $\boldsymbol{\mu}_{k+1} = \hat{\boldsymbol{\mu}}_k$ **else** $\boldsymbol{\mu}_{k+1} = \boldsymbol{\mu}_k$ **end if**

4: **Trust region update**:

if $\rho_k \leq \eta_1$ **then** $\Delta_{k+1} \in (0, \gamma\,||\hat{\boldsymbol{\mu}}_k - \boldsymbol{\mu}_k||]$ **end if**

if $\rho_k \in (\eta_1, \eta_2)$ **then** $\Delta_{k+1} \in [\gamma\,||\hat{\boldsymbol{\mu}}_k - \boldsymbol{\mu}_k||\,, \Delta_k]$ **end if**

if $\rho_k \geq \eta_2$ **then** $\Delta_{k+1} \in [\Delta_k, \Delta_{\max}]$ **end if**

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Trust region ingredients for global convergence

Approximation model

$$m_k(\boldsymbol{\mu})$$

Error indicator

$$||\nabla F(\boldsymbol{\mu}) - \nabla m_k(\boldsymbol{\mu})|| \leq \xi \varphi_k(\boldsymbol{\mu}), \qquad \xi > 0$$

Adaptivity

$$\varphi_k(\boldsymbol{\mu}_k) \leq \kappa_\varphi \min\{||\nabla m_k(\boldsymbol{\mu}_k)||\,,\, \Delta_k\}$$

Global convergence

$$\liminf_{k\to\infty} \; ||\nabla F(\boldsymbol{\mu}_k)|| = 0$$

Source of inexactness/efficiency: projection-based model reduction

- Model reduction ansatz: *state vector lies in low-dimensional subspace*

$$\boldsymbol{u} \approx \boldsymbol{\Phi} \boldsymbol{u}_r$$

  - $\boldsymbol{\Phi} = \begin{bmatrix} \boldsymbol{\phi}^1 & \cdots & \boldsymbol{\phi}^{k_{\boldsymbol{u}}} \end{bmatrix} \in \mathbb{R}^{n_{\boldsymbol{u}} \times k_{\boldsymbol{u}}}$ is the reduced (trial) basis ($n_{\boldsymbol{u}} \gg k_{\boldsymbol{u}}$)
  - $\boldsymbol{u}_r \in \mathbb{R}^{k_{\boldsymbol{u}}}$ are the reduced coordinates of $\boldsymbol{u}$

- Substitute into $\boldsymbol{r}(\boldsymbol{u}, \boldsymbol{\mu}) = 0$ and project onto columnspace of a test basis $\boldsymbol{\Phi} \in \mathbb{R}^{n_{\boldsymbol{u}} \times k_{\boldsymbol{u}}}$ to obtain a square system

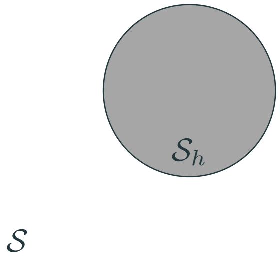
$$\boldsymbol{\Phi}^T \boldsymbol{r}(\boldsymbol{\Phi} \boldsymbol{u}_r, \boldsymbol{\mu}) = 0$$

Connection to finite element method: hierarchical subspaces

$\mathcal{S}$

- $\mathcal{S}$ - infinite-dimensional trial space

Connection to finite element method: hierarchical subspaces



- $\mathcal{S}$ - infinite-dimensional trial space
- $\mathcal{S}_h$ - (large) finite-dimensional trial space

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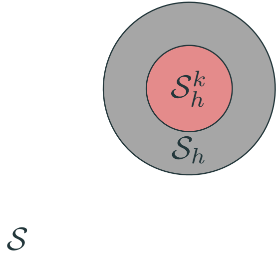
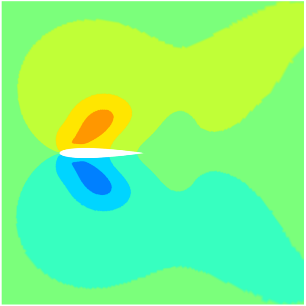
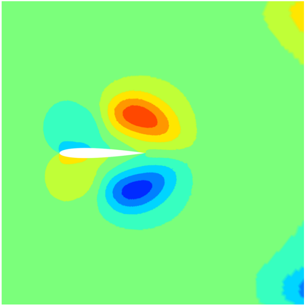
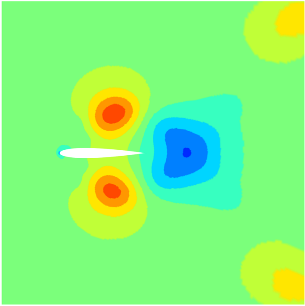


- $\mathcal{S}$ - infinite-dimensional trial space
- $\mathcal{S}_h$ - (large) finite-dimensional trial space
- $\mathcal{S}_h^k$ - (small) finite-dimensional trial space
- $\mathcal{S}_h^k \subset \mathcal{S}_h \subset \mathcal{S}$

Few global, data-driven basis functions v. many local ones

- Instead of using traditional *local* shape functions, use **global shape functions**
- Instead of a-priori, analytical shape functions, leverage data-rich computing environment by using **data-driven modes**

Trust region method: ROM approximation model

Approximation models based on reduced-order models

$$m_k(\boldsymbol{\mu}) = \mathcal{J}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}),\, \boldsymbol{\mu})$$

Error indicators from residual-based error bounds

$$\varphi_k(\boldsymbol{\mu}) = ||\boldsymbol{r}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}),\, \boldsymbol{\mu})||_{\boldsymbol{\Theta}} + \left|\left|\boldsymbol{r}^{\boldsymbol{\lambda}}(\boldsymbol{\Phi}_k \boldsymbol{u}_r(\boldsymbol{\mu}),\, \boldsymbol{\Phi}_k \boldsymbol{\lambda}_r(\boldsymbol{\mu}),\, \boldsymbol{\mu})\right|\right|_{\boldsymbol{\Theta}^{\boldsymbol{\lambda}}}$$

Adaptivity to refine basis at trust region center

$$\boldsymbol{\Phi}_k = \begin{bmatrix} \boldsymbol{u}(\boldsymbol{\mu}_k) & \boldsymbol{\lambda}(\boldsymbol{\mu}_k) & \texttt{POD}(\boldsymbol{U}_k) & \texttt{POD}(\boldsymbol{V}_k) \end{bmatrix}$$

$$\boldsymbol{U}_k = \begin{bmatrix} \boldsymbol{u}(\boldsymbol{\mu}_0) & \cdots & \boldsymbol{u}(\boldsymbol{\mu}_{k-1}) \end{bmatrix} \qquad \boldsymbol{V}_k = \begin{bmatrix} \boldsymbol{\lambda}(\boldsymbol{\mu}_0) & \cdots & \boldsymbol{\lambda}(\boldsymbol{\mu}_{k-1}) \end{bmatrix}$$

Interpolation property of minimum-residual reduced-order models $\implies \varphi_k(\boldsymbol{\mu}_k) = 0$

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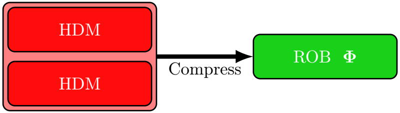
Trust region framework for optimization with ROMs

Schematic

$\boldsymbol{\mu}$-space

Breakdown of Computational Effort

Trust region framework for optimization with ROMs



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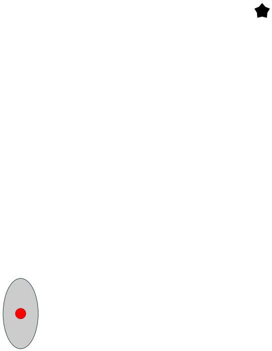

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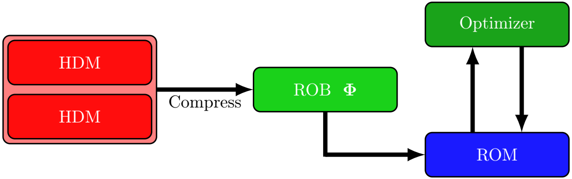

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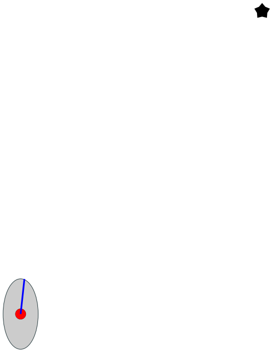

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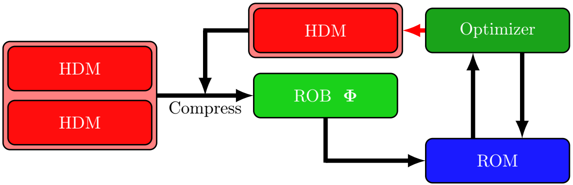

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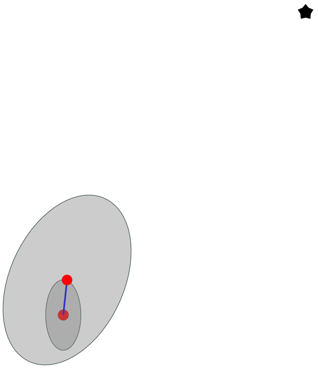

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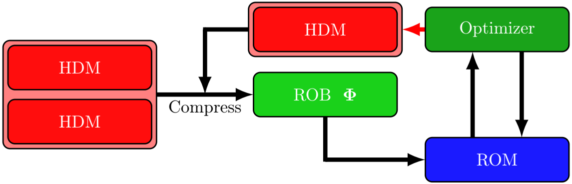

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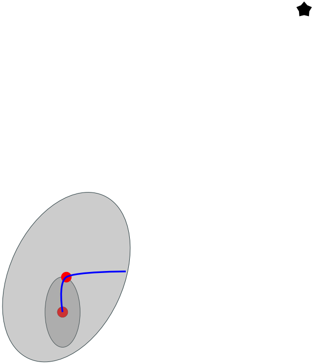

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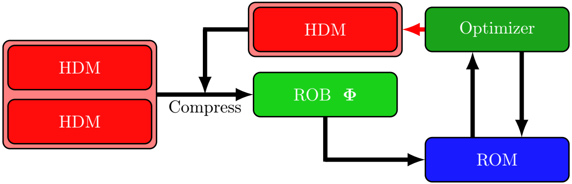

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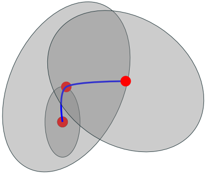

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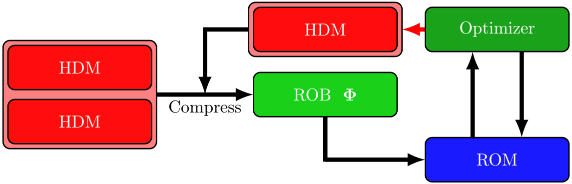

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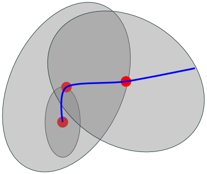

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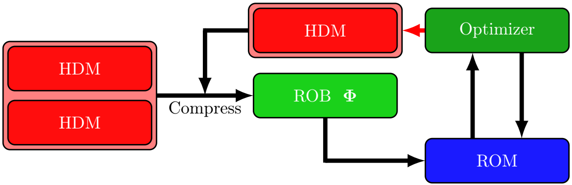

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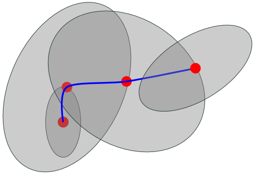

μ-space

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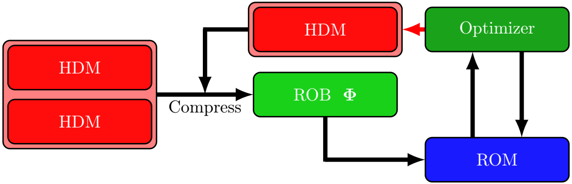

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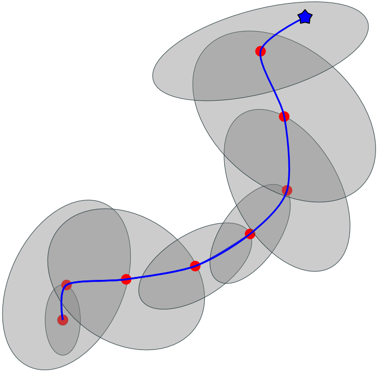
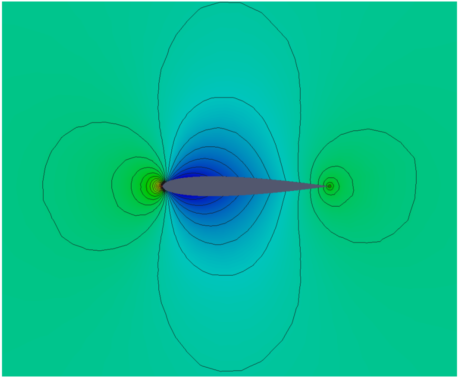


μ-space

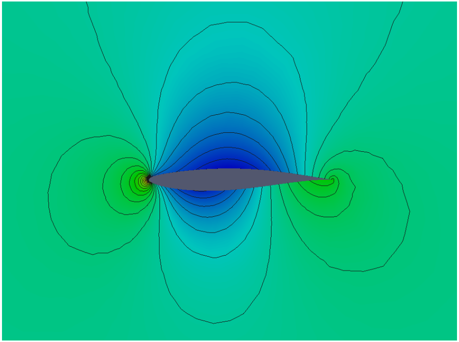
Breakdown of Computational Effort

Compressible, inviscid airfoil design

Pressure discrepancy minimization (Euler equations)



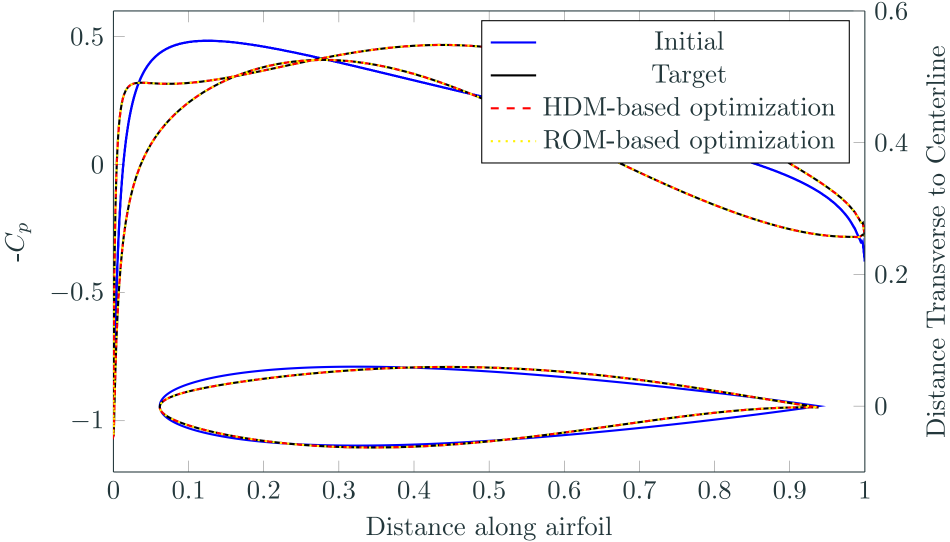
NACA0012: Initial



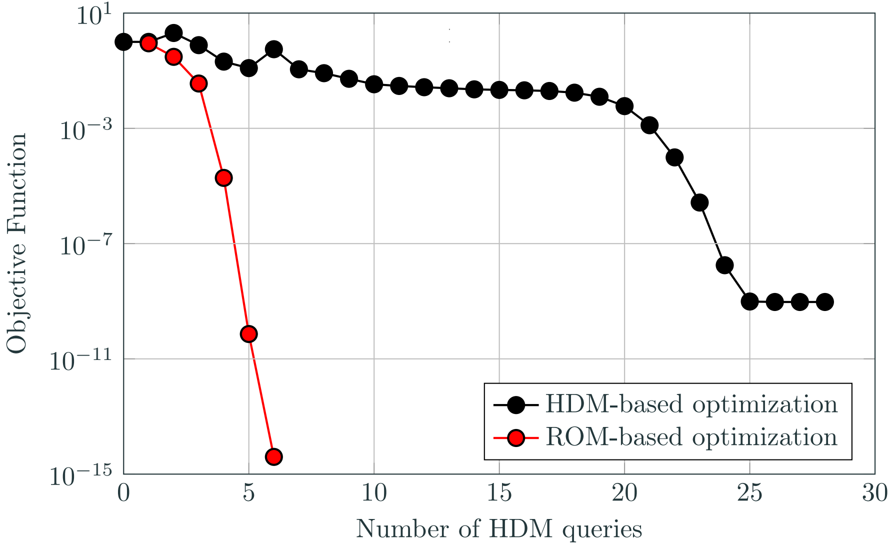
RAE2822: Target

Pressure field for airfoil configurations at $M_\infty = 0.5$, $\alpha = 0.0°$

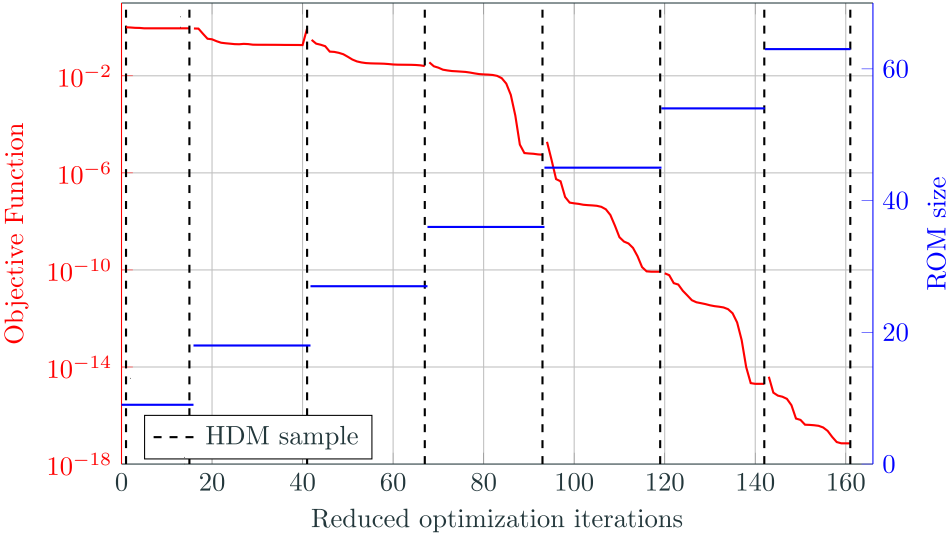
Proposed method: recovers target airfoil



Proposed method: 4× fewer HDM queries



At the cost of ROM queries

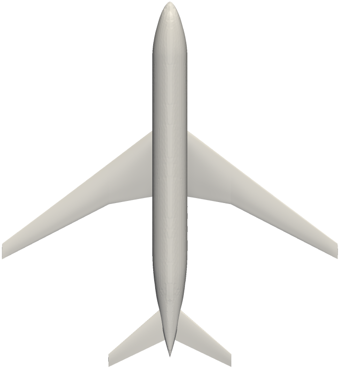


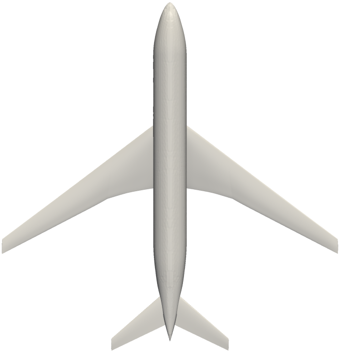
Shape optimization of aircraft in turbulent flow

$$\begin{aligned} \underset{\boldsymbol{\mu}\in\mathbb{R}^4}{\text{minimize}} \quad & -L_z(\boldsymbol{\mu})/L_x(\boldsymbol{\mu}) \\ \text{subject to} \quad & L_z(\boldsymbol{\mu}) = \bar{L}_z \end{aligned}$$

- **Flow**: $M = 0.85 \quad \alpha = 2.32^\circ \quad Re = 5 \times 10^6$
- **Equations**: RANS with Spalart-Allmaras
- **Solver**: Vertex-centered finite volume method
- **Mesh**: **11.5M** nodes, **68M** tetra, **69M** DOF

$$\boldsymbol{\mu} = [\mathbf{L} \quad r_x \quad \phi \quad r_z]$$





Shape optimization of aircraft in turbulent flow

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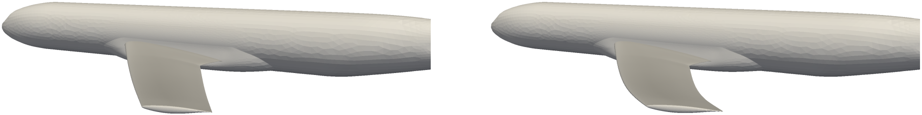

Localized sweep

Shape optimization of aircraft in turbulent flow

$$\underset{\boldsymbol{\mu}\in\mathbb{R}^4}{\text{minimize}} \quad -L_z(\boldsymbol{\mu})/L_x(\boldsymbol{\mu})$$
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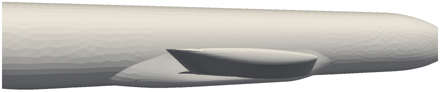
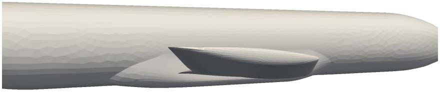
$$\boldsymbol{\mu} = [L \quad r_x \quad \boldsymbol{\phi} \quad r_z]$$





Twist

Shape optimization of aircraft in turbulent flow

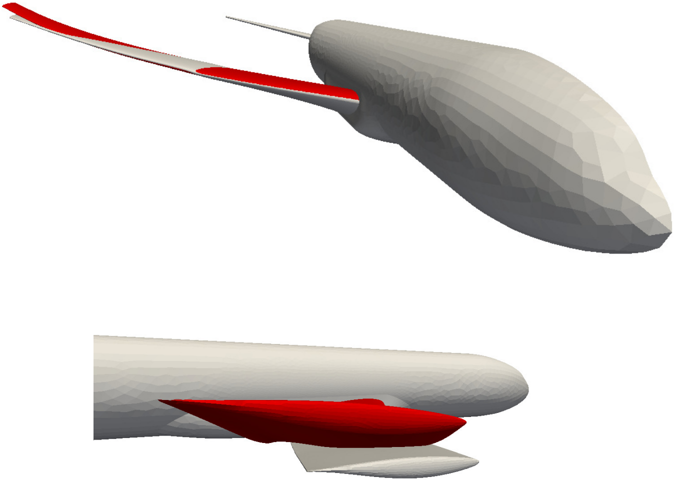
$$\underset{\boldsymbol{\mu}\in\mathbb{R}^4}{\text{minimize}} \quad -L_z(\boldsymbol{\mu})/L_x(\boldsymbol{\mu})$$
$$\text{subject to} \quad L_z(\boldsymbol{\mu}) = \bar{L}_z$$

- **Flow**: $M = 0.85 \quad \alpha = 2.32^\circ \quad Re = 5 \times 10^6$
- **Equations**: RANS with Spalart-Allmaras
- **Solver**: Vertex-centered finite volume method
- **Mesh**: **11.5M** nodes, **68M** tetra, **69M** DOF

$$\boldsymbol{\mu} = [L \quad r_x \quad \phi \quad \mathbf{r_z}]$$

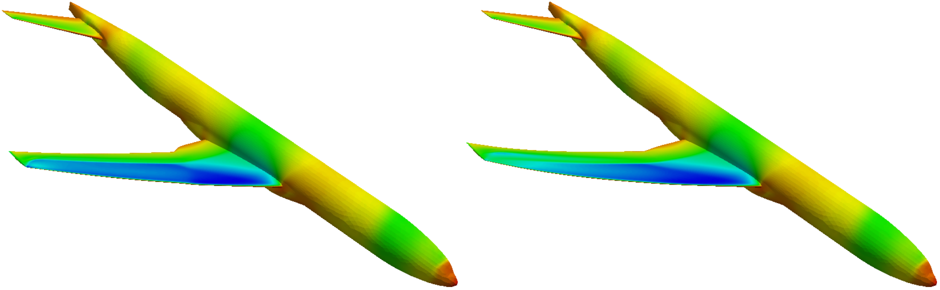
Localized dihedral

Optimized shape: reduction in 2.2 drag counts



Baseline (gray) and optimized shape (red) – 2× magnification

Optimized shape: reduction in 2.2 drag counts



Baseline (left) and optimized (right) shape – colored by C_p

Performance: ROM-TR method obtains same solution (to 4 digits of accuracy) as HDM-only optimization and only requires about 60% of the computation time.

Conclusion: Very promising results considering ROMs have notoriously poor prediction capabilities for problems with moving shocks/discontinuities.

Application to Bayesian parameter estimation

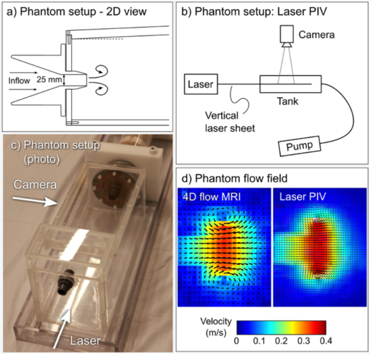
Enhance numerical simulation with noisy solution data

Let $\boldsymbol{z}$ denote noisy solution measurements that can be expressed as a function of the simulation parameters $\boldsymbol{\mu}$ and noise term $\boldsymbol{\epsilon}$ (known distribution) as

$$\boldsymbol{z} = \boldsymbol{h}(\boldsymbol{\mu}) + \boldsymbol{\epsilon},$$

where $\boldsymbol{h}$ is a function that maps simulation parameters to solution observations.

Example: Magnetic resonance imaging



Experimental setup

Noisy, low-resolution MRI data

Bayesian setting for parameter estimation

We want to estimate the probability distribution over the parameter space, given the data we have observed, i.e., the posterior $p(\boldsymbol{\mu}|\boldsymbol{z})$

$$p(\boldsymbol{\mu}|\boldsymbol{z}) \propto p(\boldsymbol{\mu})p(\boldsymbol{z}|\boldsymbol{\mu}),$$

where $p(\boldsymbol{\mu})$ is the prior distribution and the distribution $p(\boldsymbol{z}|\boldsymbol{\mu})$ can be inferred directly from our ansatz regarding the nature of the data ($\boldsymbol{z} = \boldsymbol{h}(\boldsymbol{\mu}) + \boldsymbol{\epsilon}$).

Importance sampling: empirical estimate of $p(\boldsymbol{\mu}|\boldsymbol{z})$ (and related statistics) where each sample assigned weights $(\boldsymbol{\mu}_j, w_j)$ to focus samples on important regions of parameter space, e.g., the expectation is approximated via the M-sample estimate

$$\mathbb{E}_M[\boldsymbol{g}(\boldsymbol{\mu})] = \sum_{j=1}^{M} \hat{w}_j \boldsymbol{g}(\boldsymbol{\mu}_j),$$

where $\hat{w}_j = \frac{w_j}{\sum_{j=1}^{M} w_j}$.

Parameter estimation via implicit sampling

Implicit sampling

Special case of importance sampling where samples computed by solving implicit equation [Morzfeld et al., 2015]

1) Find maximum a posteriori (MAP) point, $\boldsymbol{\mu}^*$, by maximizing

$$F(\boldsymbol{\mu}) = -\log p(\boldsymbol{\mu}) p(\boldsymbol{z}|\boldsymbol{\mu})$$

   $\rightarrow$ PDE-constrained optimization : $p(\boldsymbol{z}|\boldsymbol{\mu})$ requires solution of the PDE

2) Compute Hessian of F at $\boldsymbol{\mu}^*$, denoted $\boldsymbol{H}$
3) Implicit sampling in M random directions $\boldsymbol{\xi}_j$

$$F(\boldsymbol{\mu}^* + \lambda \boldsymbol{\xi}_j) - \phi = \frac{1}{2} \boldsymbol{\xi}_j^T \boldsymbol{H} \boldsymbol{\xi}_j$$

Acceleration using reduced-order models

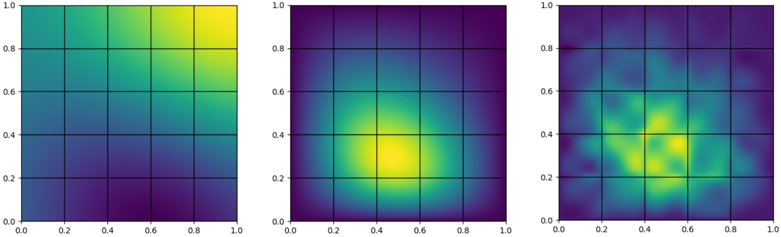
1) Accelerate optimization using trust-region framework and ROMs $\rightarrow \boldsymbol{\mu}^*, \boldsymbol{\Phi}$
2) Approximate Hessian using ROM and finite differences
3) Use ROM for implicit sampling

Parameter estimation: elliptic PDE

Consider the elliptic PDE, often used to model subsurface flow,

$$\begin{aligned} -\nabla \cdot (\kappa \nabla p) &= g \quad \text{in } \Omega \\ p &= h \quad \text{on } \partial\Omega, \end{aligned}$$

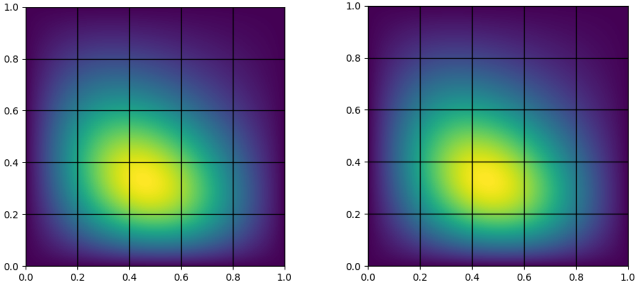
where p is the (partially observed) pressure field and κ is the (unknown) permeability. Pressure at 25% of FEM nodes is observed and the noise added is $\mathcal{N}(0, 0.3p_{\max})$.



True permeability (*left*), true pressure (*center*), and observed pressure (*right*).

Goal: *estimate the probability distribution of* κ *given the observations of* p

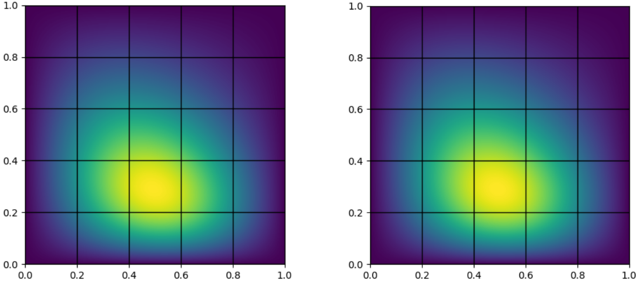
Computation of MAP point: HDM-only vs. HDM-ROM



MAP point: only HDM evaluations (*left*) and the ROM trust region method (*right*).

Performance:

	HDM-only	ROM-TR
HDM primal	27	8
HDM sensitivity	27	8
ROM primal	0	30
ROM sensitivity	0	30



Mean of posterior: only HDM evaluations (*left*) and the ROM trust region method (*right*).

Performance:

	Hessian evaluation		**Implicit sampling**	
	HDM-only	ROM-TR	HDM-only	ROM-TR
HDM primal	12	0	1799	0
HDM sensitivity	12	0	1799	0
ROM primal	0	12	0	1781
ROM sensitivity	0	12	0	1781

Leveraging inexactness to accelerate PDE-constrained optimization

- Framework introduced to accelerate PDE-constrained optimization
  - Adaptive *model reduction*
  - *Partially converged* primal and adjoint solutions
- Inexactness **managed** with flexible **trust region** method
- Applied to variety of problems in computational mechanics and outperforms standard methods
  - **5**× speedup: *subsonic* shape optimization of airfoil
  - **1.6**× speedup: *transonic* shape design of aircraft
- Extended/applied to accelerate **Bayesian parameter estimation**
  - Use ROM-TR method to find MAP point $\boldsymbol{\mu}^*$
  - Use reduced basis built during optimization to approximate Hessian at $\boldsymbol{\mu}^*$
  - Re-cast sampling procedure as optimization problem and apply ROM-TR

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