Adjoint-based PDE-constrained optimization using globally high-order numerical discretizations

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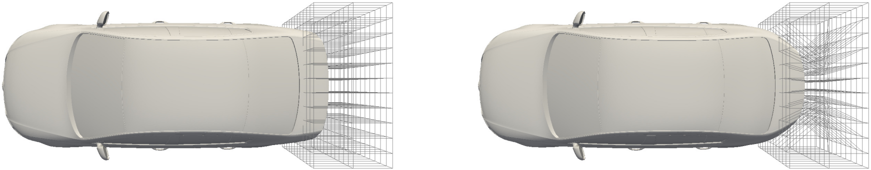
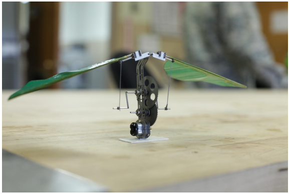
PDE optimization is ubiquitous in science and engineering

Design: Find system that optimizes performance metric, satisfies constraints



Aerodynamic shape design of automobile



Optimal flapping motion of micro aerial vehicle

Control, inverse problems

Unsteady PDE-constrained optimization formulation

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

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

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

High-order discretization of PDE-constrained optimization

- *Continuous* PDE-constrained optimization problem

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

- *Fully discrete* PDE-constrained optimization problem

$$\begin{aligned} \underset{\substack{\boldsymbol{u}_0,\ \dots,\ \boldsymbol{u}_{N_t} \in \mathbb{R}^{N_{\boldsymbol{u}}}, \\ \boldsymbol{k}_{1,1},\ \dots,\ \boldsymbol{k}_{N_t,s} \in \mathbb{R}^{N_{\boldsymbol{u}}}, \\ \boldsymbol{\mu} \in \mathbb{R}^{n_{\boldsymbol{\mu}}}}}{\text{minimize}} \quad & J(\boldsymbol{u}_0,\ \dots,\ \boldsymbol{u}_{N_t},\ \boldsymbol{k}_{1,1},\ \dots,\ \boldsymbol{k}_{N_t,s},\ \boldsymbol{\mu}) \\ \text{subject to} \quad & \mathbf{C}(\boldsymbol{u}_0,\ \dots,\ \boldsymbol{u}_{N_t},\ \boldsymbol{k}_{1,1},\ \dots,\ \boldsymbol{k}_{N_t,s},\ \boldsymbol{\mu}) \leq 0 \\ & \boldsymbol{u}_0 - \boldsymbol{g}(\boldsymbol{\mu}) = 0 \\ & \boldsymbol{u}_n - \boldsymbol{u}_{n-1} - \sum_{i=1}^{s} b_i \boldsymbol{k}_{n,i} = 0 \\ & \boldsymbol{M}\boldsymbol{k}_{n,i} - \Delta t_n \boldsymbol{r}\left(\boldsymbol{u}_{n,i},\ \boldsymbol{\mu},\ t_{n,i}\right) = 0 \end{aligned}$$

Adjoint method to efficiently compute gradients of QoI

- Consider the *fully discrete* output functional $F(\boldsymbol{u}_n, \boldsymbol{k}_{n,i}, \boldsymbol{\mu})$
  - Represents either the **objective** function or a **constraint**
- The *total derivative* with respect to the parameters $\boldsymbol{\mu}$, required in the context of gradient-based optimization, takes the form

$$\frac{\mathrm{d}F}{\mathrm{d}\boldsymbol{\mu}} = \frac{\partial F}{\partial \boldsymbol{\mu}} + \sum_{n=0}^{N_t} \frac{\partial F}{\partial \boldsymbol{u}_n} \frac{\partial \boldsymbol{u}_n}{\partial \boldsymbol{\mu}} + \sum_{n=1}^{N_t} \sum_{i=1}^{s} \frac{\partial F}{\partial \boldsymbol{k}_{n,i}} \frac{\partial \boldsymbol{k}_{n,i}}{\partial \boldsymbol{\mu}}$$

- The sensitivities, $\frac{\partial \boldsymbol{u}_n}{\partial \boldsymbol{\mu}}$ and $\frac{\partial \boldsymbol{k}_{n,i}}{\partial \boldsymbol{\mu}}$, are expensive to compute, requiring the solution of $n_{\boldsymbol{\mu}}$ linear evolution equations
- **Adjoint method**: alternative method for computing $\frac{\mathrm{d}F}{\mathrm{d}\boldsymbol{\mu}}$ that require one linear evolution equation for each quantity of interest, F

Dissection of fully discrete adjoint equations

- **Linear** evolution equations solved **backward** in time
- **Primal** state/stage, $\boldsymbol{u}_{n,i}$ required at each state/stage of dual problem
- Heavily dependent on **chosen ouput**

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

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

$$\boldsymbol{M}^T \boldsymbol{\kappa}_{n,i} = \frac{\partial F}{\partial \boldsymbol{u}_{N_t}}^T + b_i \boldsymbol{\lambda}_n + \sum_{j=i}^{s} a_{ji} \Delta t_n \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{u}} \left(\boldsymbol{u}_{n,j},\ \boldsymbol{\mu},\ t_{n-1} + c_j \Delta t_n\right)^T \boldsymbol{\kappa}_{n,j}$$

- Gradient reconstruction via dual variables

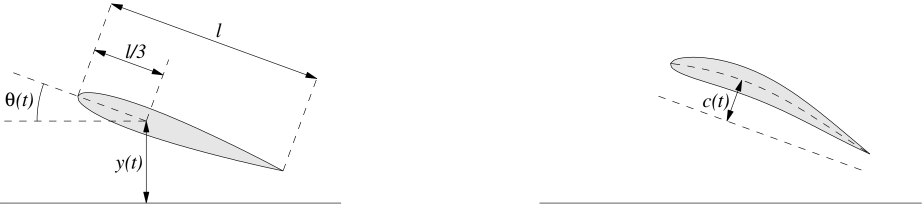
$$\frac{\mathrm{d}F}{\mathrm{d}\boldsymbol{\mu}} = \frac{\partial F}{\partial \boldsymbol{\mu}} + \boldsymbol{\lambda}_0{}^T \frac{\partial \boldsymbol{g}}{\partial \boldsymbol{\mu}}(\boldsymbol{\mu}) + \sum_{n=1}^{N_t} \Delta t_n \sum_{i=1}^{s} \boldsymbol{\kappa}_{n,i}{}^T \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{\mu}}(\boldsymbol{u}_{n,i},\ \boldsymbol{\mu},\ t_{n,i})$$

[Zahr and Persson, 2016]

Energetically optimal flapping under x-impulse constraint

$$
\begin{aligned}
\underset{\boldsymbol{\mu}}{\text{minimize}} \quad & -\int_{2T}^{3T}\int_{\boldsymbol{\Gamma}} \boldsymbol{f}\cdot\boldsymbol{v}\,dS\,dt \\
\text{subject to} \quad & \int_{2T}^{3T}\int_{\boldsymbol{\Gamma}} \boldsymbol{f}\cdot\boldsymbol{e}_1\,dS\,dt = q \\
& \boldsymbol{U}(\boldsymbol{x},0) = \boldsymbol{g}(\boldsymbol{x}) \\
& \frac{\partial \boldsymbol{U}}{\partial t} + \nabla\cdot\boldsymbol{F}(\boldsymbol{U},\nabla\boldsymbol{U}) = 0
\end{aligned}
$$

- Isentropic, compressible, Navier-Stokes
- Re $=1000$, M $=0.2$
- $y(t)$, $\theta(t)$, $c(t)$ parametrized via periodic cubic splines
- Black-box optimizer: SNOPT



Airfoil schematic, kinematic description

Optimal control, time-morphed geometry

Optimal Rigid Body Motion (RBM) and Time-Morphed Geometry (TMG),
x*-impulse* $= -2.5$

Energy = 9.4096	Energy = 4.9476	Energy = 4.6182
x-impulse = -0.1766	x-impulse = -2.500	x-impulse = -2.500
Initial Guess	Optimal RBM $J_x = -2.5$	Optimal RBM/TMG $J_x = -2.5$

Energetically optimal flapping in three-dimensions

Energy = 1.4459e-01
Thrust = -1.1192e-01

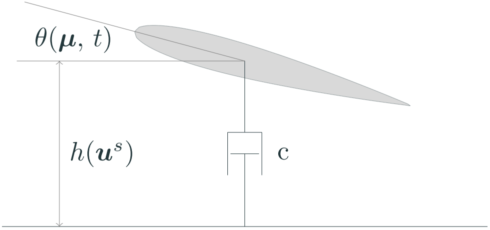
Energy = 3.1378e-01
Thrust = 0.0000e+00

Optimal energy harvesting from foil-damper system

Goal: Maximize energy harvested from foil-damper system

$$\underset{\boldsymbol{\mu}}{\text{maximize}} \quad \frac{1}{T}\int_0^T \left(c\dot{h}^2(\boldsymbol{u}^s) - M_z(\boldsymbol{u}^f)\dot{\theta}(\boldsymbol{\mu},\, t)\right) dt$$

- Fluid: Isentropic Navier-Stokes on deforming domain (ALE)
- Structure: Force balance in y-direction between foil and damper
- Motion driven by *imposed* $\theta(\boldsymbol{\mu},\, t) = \mu_1 \cos(2\pi f t)$; $\mu_1 \in (-45°,\, 45°)$



$\mu_1^* = 45°$

Data assimilation: inverse problem in medical imaging

Goal: Determine the boundary conditions that produces a high-resolution flow that matches low-resolution flow measurements ($\boldsymbol{d}^*$)

$$
\begin{aligned}
\underset{\boldsymbol{\mu}}{\text{minimize}} \quad & \frac{1}{2}|\boldsymbol{d}(\boldsymbol{U}) - \boldsymbol{d}^*|^2 \\
\text{subject to} \quad & \frac{\partial \boldsymbol{U}}{\partial t} + \nabla \cdot \boldsymbol{F}(\boldsymbol{U}, \nabla \boldsymbol{U}) = 0 \qquad \text{in } \Omega \\
& \boldsymbol{U} = \boldsymbol{\mu} \qquad \text{on } \Gamma
\end{aligned}
$$

Data assimilation: inverse problem in medical imaging

True flow

Data

Reconstructed flow

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