High-Order, Time-Dependent Aerodynamic Optimization using a Discontinuous Galerkin Discretization of the Navier-Stokes Equations

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Thought Experiment: Which motion ...

- Has time-averaged x-force identically equal to 0?
- Requires least energy to perform?

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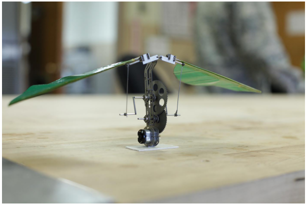
Energy = 9.4096	Energy = 0.45695	Energy = 4.9475
x-force = -0.8830	x-force = 0.000	x-force = -12.50

Real-World Application: Micro Aerial Vehicles (MAV)

- Unmanned flying vehicle
  - usually flapping propulsion system
  - wingspan between 7.4cm and 15cm
  - speed between $\leq$ 15m/s
- Military applications
  - surveillance, reconnaissance
  - quiet, resemble small bird from distance
- Civilian applications
  - Crowd monitoring, survivor search, pipeline inspection
- Difficulties
  - Thrust and lift requirements
  - Structural constraints
  - Stability and control considerations

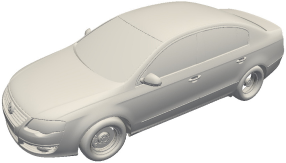


Micro Aerial Vehicle

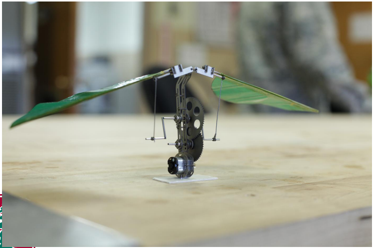
Bumblebee MAV (USAF 2008)

Time-Dependent PDE-Constrained Optimization

- Optimization of systems that are inherently dynamic or without a steady-state solution
- Introduction of **fully discrete adjoint method** emanating from **high-order** discretization of governing equations
- Coupled with numerical optimization
- **Time-periodicity** constraints

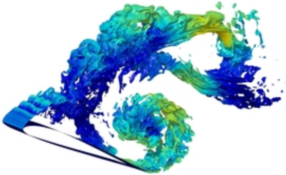


Volkswagen Passat



Micro Aerial Vehicle

Vertical Windmill



LES Flow past Airfoil

Abstract Formulation of Problem of Interest

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

High-Order Discretization of PDE-Constrained Optimization

- *Continuous* PDE-constrained optimization problem

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

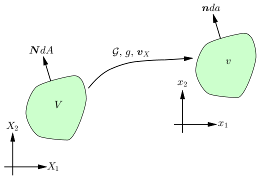
- *Fully discrete* PDE-constrained optimization problem

$$\begin{aligned} \underset{\substack{\boldsymbol{u}^{(0)},\,\ldots,\,\boldsymbol{u}^{(N_t)}\in\mathbb{R}^{N_{\boldsymbol{u}}},\\ \boldsymbol{k}_1^{(1)},\,\ldots,\,\boldsymbol{k}_s^{(N_t)}\in\mathbb{R}^{N_{\boldsymbol{u}}},\\ \boldsymbol{\mu}\in\mathbb{R}^{n_{\boldsymbol{\mu}}}}}{\text{minimize}} \quad & J(\boldsymbol{u}^{(0)},\ \ldots,\ \boldsymbol{u}^{(N_t)},\ \boldsymbol{k}_1^{(1)},\ \ldots,\ \boldsymbol{k}_s^{(N_t)},\ \boldsymbol{\mu}) \\ \text{subject to} \quad & \mathbf{C}(\boldsymbol{u}^{(0)},\ \ldots,\ \boldsymbol{u}^{(N_t)},\ \boldsymbol{k}_1^{(1)},\ \ldots,\ \boldsymbol{k}_s^{(N_t)},\ \boldsymbol{\mu}) \leq 0 \\ & \boldsymbol{u}^{(0)} - \boldsymbol{u}_0(\boldsymbol{\mu}) = 0 \\ & \boldsymbol{u}^{(n)} - \boldsymbol{u}^{(n-1)} + \sum_{i=1}^{s} b_i \boldsymbol{k}_i^{(n)} = 0 \\ & \mathbb{M}\boldsymbol{k}_i^{(n)} - \Delta t_n \boldsymbol{r}\left(\boldsymbol{u}_i^{(n)},\ \boldsymbol{\mu},\ t_i^{(n-1)}\right) = 0 \end{aligned}$$

Highlights of Globally High-Order Discretization

- **Arbitrary Lagrangian-Eulerian** Formulation: Map, $\mathcal{G}(\cdot, \boldsymbol{\mu}, t)$, from physical $v(\boldsymbol{\mu}, t)$ to reference V

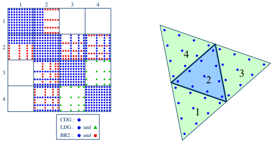
$$\left.\frac{\partial \boldsymbol{U_X}}{\partial t}\right|_{\boldsymbol{X}} + \nabla_{\boldsymbol{X}} \cdot \boldsymbol{F_X}(\boldsymbol{U_X},\ \nabla_{\boldsymbol{X}} \boldsymbol{U_X}) = 0$$



Mapping-Based ALE

- **Space Discretization**: Discontinuous Galerkin

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



DG Discretization

- **Time Discretization**: Diagonally Implicit RK

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

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

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

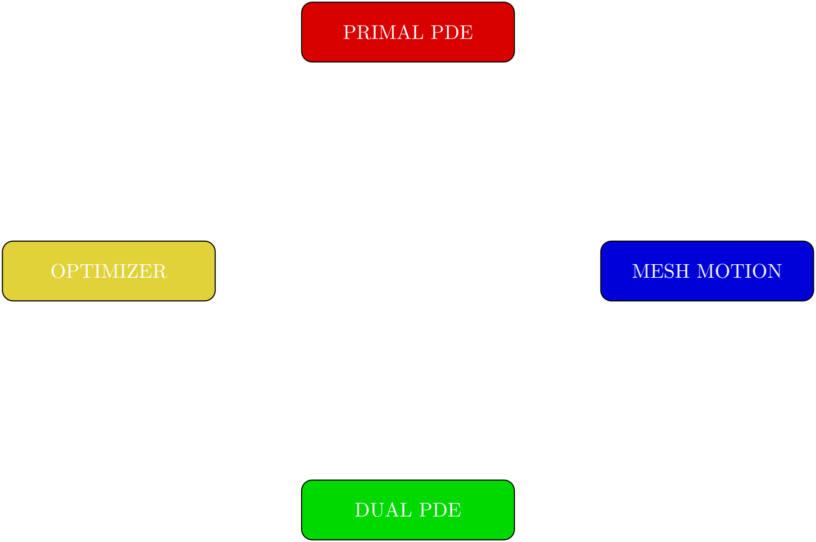
Butcher Tableau for DIRK

- **Quantity of Interest**: Solver-consistent

$$F(\boldsymbol{u}^{(0)}, \ldots, \boldsymbol{u}^{(N_t)}, \boldsymbol{k}_1^{(1)}, \ldots, \boldsymbol{k}_s^{(N_t)})$$

Generalized Reduced-Gradient Approach - Schematic

Optimizer drives, Primal returns QoI values, Dual returns QoI gradients



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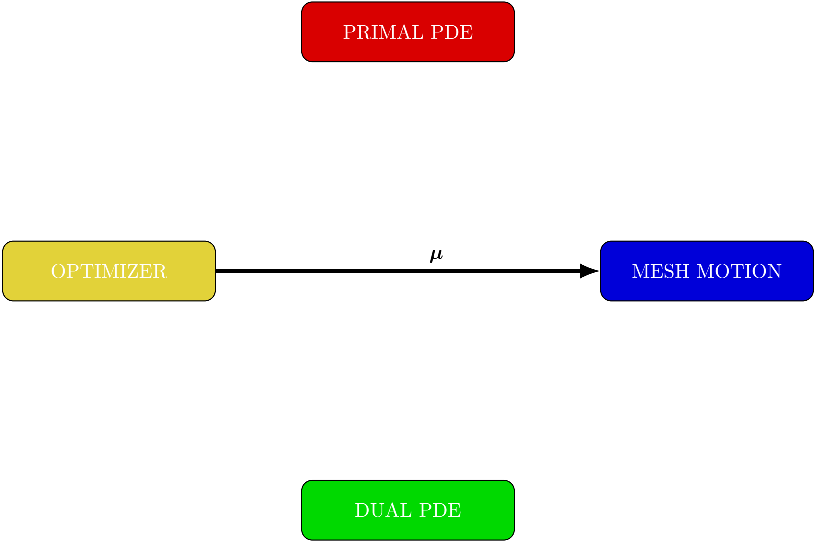

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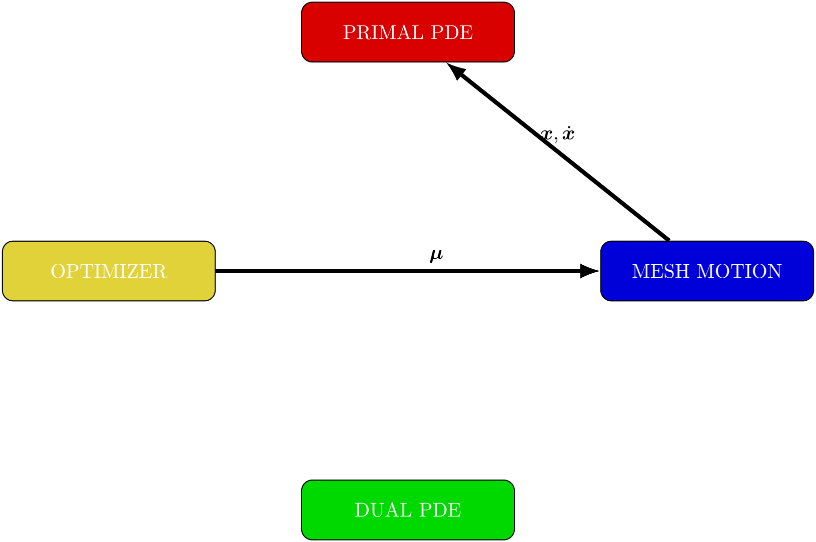

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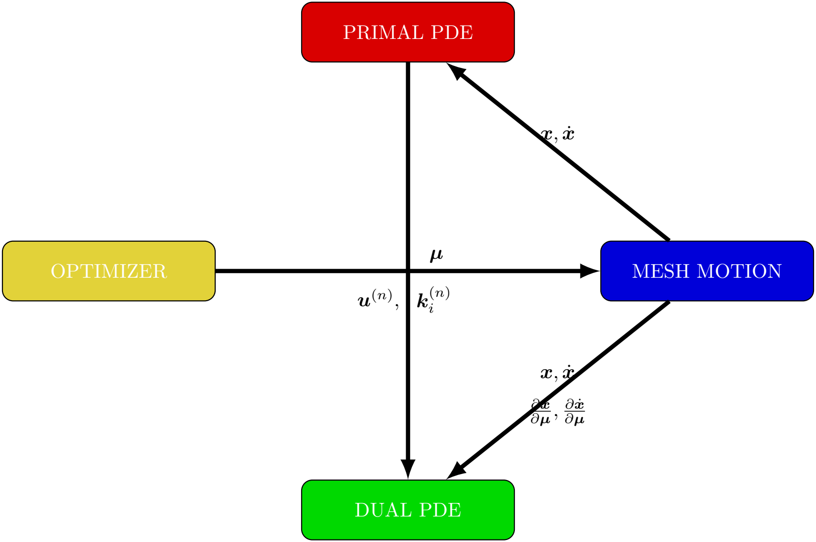
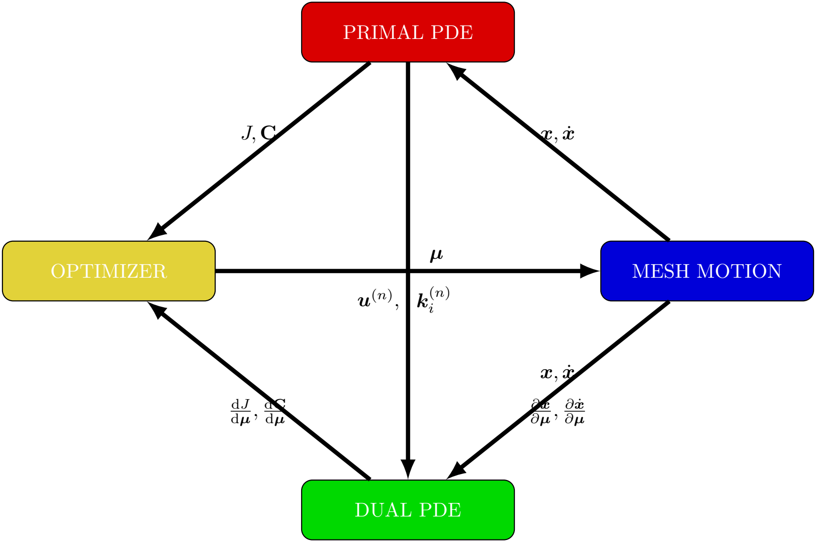


Generalized Reduced-Gradient Approach - Schematic

Optimizer drives, Primal returns QoI values, Dual returns QoI gradients



Adjoint Method to Compute QoI Gradients

- Consider the *fully discrete* output functional $F(\boldsymbol{u}^{(n)}, \boldsymbol{k}_i^{(n)}, \boldsymbol{\mu})$
  - 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

$$\frac{\mathrm{d}F}{\mathrm{d}\boldsymbol{\mu}} = \frac{\partial F}{\partial \boldsymbol{\mu}} + \sum_{n=0}^{N_t} \frac{\partial F}{\partial \boldsymbol{u}^{(n)}} \frac{\partial \boldsymbol{u}^{(n)}}{\partial \boldsymbol{\mu}} + \sum_{n=1}^{N_t} \sum_{i=1}^{s} \frac{\partial F}{\partial \boldsymbol{k}_i^{(n)}} \frac{\partial \boldsymbol{k}_i^{(n)}}{\partial \boldsymbol{\mu}}$$

- The sensitivities, $\frac{\partial \boldsymbol{u}^{(n)}}{\partial \boldsymbol{\mu}}$ and $\frac{\partial \boldsymbol{k}_i^{(n)}}{\partial \boldsymbol{\mu}}$, 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 evoluation equation for each quantity of interest, F

Fully Discrete Adjoint Equations: Dissection

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

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

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

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

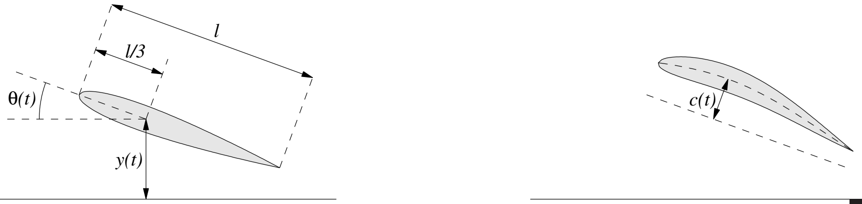
- Gradient reconstruction via dual variables

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

Energetically Optimal Flapping under x-Impulse Constraint

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

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



Airfoil schematic, kinematic description

Optimal Control - Fixed Shape

Fixed Shape, Optimal Rigid Body Motion (RBM), Varied x-Impulse

Initial Guess	Optimal RBM, $J_x = 0.0$	Optimal RBM, $J_x = -2.5$
Energy = 9.4096	Energy = 0.45695	Energy = 4.9475
x-impulse = -0.1766	x-impulse = 0.000	x-impulse = -2.500

Initial Guess

Optimal RBM
$J_x = 0.0$

Optimal RBM
$J_x = -2.5$

Optimal Control, Time-Morphed Geometry

Optimal Rigid Body Motion (RBM) and Time-Morphed Geometry (TMG), Varied x-Impulse

Energy $=$ 9.4096	Energy $=$ 0.45027	Energy $=$ 4.6182
x-impulse $=$ -0.1766	x-impulse $=$ 0.000	x-impulse $=$ -2.500
Initial Guess	Optimal RBM/TMG $J_x = 0.0$	Optimal RBM/TMG $J_x = -2.5$

Optimal Control, Time-Morphed Geometry

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

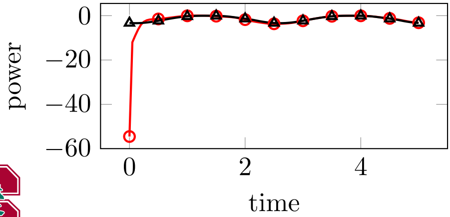
Initial Guess	Optimal RBM	Optimal RBM/TMG
Energy $= 9.4096$	Energy $= 4.9476$	Energy $= 4.6182$
x-impulse = -0.1766	x-impulse = -2.500	x-impulse = -2.500
	$J_x = -2.5$	$J_x = -2.5$

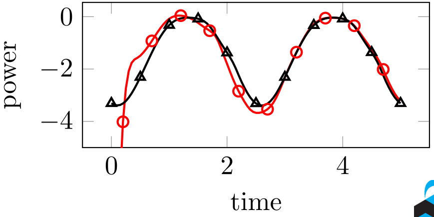
Time-Periodic Solutions Desired when Optimizing Cyclic Motion

- To properly optimize a cyclic, or periodic problem, need to simulate a **representative** period
- Necessary to avoid transients that will impact quantity of interest and may cause simulation to crash
- **Task**: Find initial condition, $\boldsymbol{u}_0$, such that flow is periodic, i.e. $\boldsymbol{u}^{(N_t)} = \boldsymbol{u}_0$

Time-Periodic Solutions Desired when Optimizing Cyclic Motion

Vorticity around airfoil with flow initialized from steady-state (left) and time-periodic flow (right)





Time history of power on airfoil of flow initialized from steady-state (—○—) and from a time-periodic solution (—△—)

Definition of Time-Periodic Solution of Fully Discrete PDE

- Recall fully discrete conservation law

$$\begin{aligned}
\boldsymbol{u}^{(0)} &= \boldsymbol{u}_0(\boldsymbol{\mu}) \\
\boldsymbol{u}^{(n)} &= \boldsymbol{u}^{(n-1)} + \sum_{i=1}^{s} b_i \boldsymbol{k}_i^{(n)} \\
\boldsymbol{u}_i^{(n)} &= \boldsymbol{u}^{(n-1)} + \sum_{j=1}^{i} a_{ij} \boldsymbol{k}_j^{(n)} \\
\mathbb{M}\boldsymbol{k}_i^{(n)} &= \Delta t_n \boldsymbol{r}\left(\boldsymbol{u}_i^{(n)},\ \boldsymbol{\mu},\ t_{n-1} + c_i \Delta t_n\right)
\end{aligned}$$

- Discrete time-periodicity is defined as

$$\boldsymbol{u}^{(N_t)}(\boldsymbol{u}_0) = \boldsymbol{u}_0$$

Time-Periodicity Constraints in PDE-Constrained Optimization

Recall *fully discrete* PDE-constrained optimization problem

$$
\begin{aligned}
\underset{\substack{\boldsymbol{u}^{(0)},\ \dots,\ \boldsymbol{u}^{(N_t)} \in \mathbb{R}^{N_{\boldsymbol{u}}},\\ \boldsymbol{k}_1^{(1)},\ \dots,\ \boldsymbol{k}_s^{(N_t)} \in \mathbb{R}^{N_{\boldsymbol{u}}},\\ \boldsymbol{\mu} \in \mathbb{R}^{n_{\boldsymbol{\mu}}}}}{\text{minimize}} \quad & J(\boldsymbol{u}^{(0)},\ \dots,\ \boldsymbol{u}^{(N_t)},\ \boldsymbol{k}_1^{(1)},\ \dots,\ \boldsymbol{k}_s^{(N_t)},\ \boldsymbol{\mu}) \\
\text{subject to} \quad & \mathbf{C}(\boldsymbol{u}^{(0)},\ \dots,\ \boldsymbol{u}^{(N_t)},\ \boldsymbol{k}_1^{(1)},\ \dots,\ \boldsymbol{k}_s^{(N_t)},\ \boldsymbol{\mu}) \leq 0 \\
& \boldsymbol{u}^{(0)} - \boldsymbol{u}_0(\boldsymbol{\mu}) = 0 \\
& \boldsymbol{u}^{(n)} - \boldsymbol{u}^{(n-1)} + \sum_{i=1}^{s} b_i \boldsymbol{k}_i^{(n)} = 0 \\
& \mathbb{M}\boldsymbol{k}_i^{(n)} - \Delta t_n \boldsymbol{r}\left(\boldsymbol{u}_i^{(n)},\ \boldsymbol{\mu},\ t_i^{(n-1)}\right) = 0
\end{aligned}
$$

Time-Periodicity Constraints in PDE-Constrained Optimization

Slight modification leads to fully discrete periodic PDE-constrained optimization

$$\begin{aligned}
\underset{\substack{\boldsymbol{u}^{(0)},\,\ldots,\,\boldsymbol{u}^{(N_t)}\in\mathbb{R}^{N_{\boldsymbol{u}}},\\ \boldsymbol{k}_1^{(1)},\,\ldots,\,\boldsymbol{k}_s^{(N_t)}\in\mathbb{R}^{N_{\boldsymbol{u}}},\\ \boldsymbol{\mu}\in\mathbb{R}^{n_{\boldsymbol{\mu}}}}}{\text{minimize}} \quad & J(\boldsymbol{u}^{(0)},\,\ldots,\,\boldsymbol{u}^{(N_t)},\,\boldsymbol{k}_1^{(1)},\,\ldots,\,\boldsymbol{k}_s^{(N_t)},\,\boldsymbol{\mu}) \\
\text{subject to} \quad & \mathbf{C}(\boldsymbol{u}^{(0)},\,\ldots,\,\boldsymbol{u}^{(N_t)},\,\boldsymbol{k}_1^{(1)},\,\ldots,\,\boldsymbol{k}_s^{(N_t)},\,\boldsymbol{\mu}) \leq 0 \\
& \boldsymbol{u}^{(0)} - \boldsymbol{u}^{(N_t)} = 0 \\
& \boldsymbol{u}^{(n)} - \boldsymbol{u}^{(n-1)} + \sum_{i=1}^{s} b_i \boldsymbol{k}_i^{(n)} = 0 \\
& \mathbb{M}\boldsymbol{k}_i^{(n)} - \Delta t_n \boldsymbol{r}\left(\boldsymbol{u}_i^{(n)},\,\boldsymbol{\mu},\,t_i^{(n-1)}\right) = 0
\end{aligned}$$

Adjoint Method for Periodic PDE-Constrained Optimization

- Following identical procedure as for non-periodic case, the adjoint equations corresponding to the periodic conservation law are

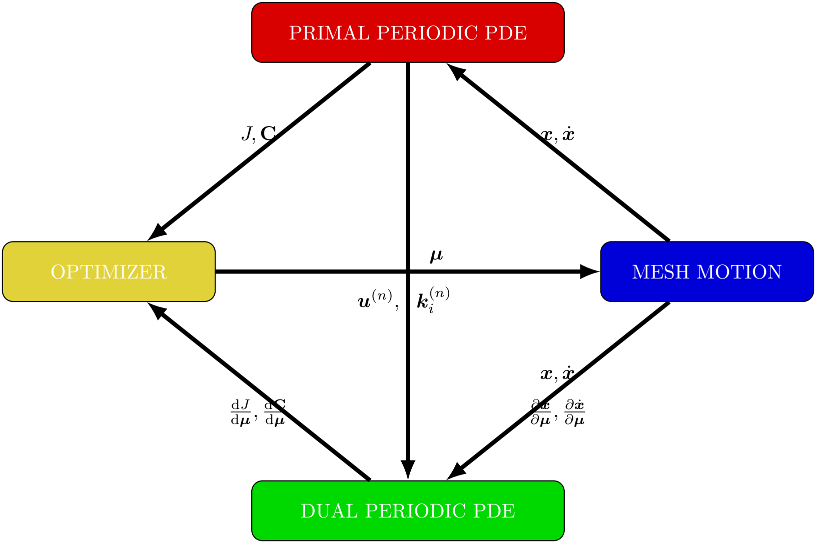
$$\boldsymbol{\lambda}^{(N_t)} = \color{red}{\boldsymbol{\lambda}^{(0)}} \color{black}{+ \frac{\partial F}{\partial \boldsymbol{u}^{(N_t)}}^T}$$

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

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

- Dual problem is also periodic
- Solve *linear, periodic* problem using Krylov shooting method

Generalized Reduced-Gradient Approach - Periodic Case



Energetically Optimal Flapping: x-Impulse, Time-Periodicity Constraint

$$\begin{aligned} \underset{\boldsymbol{\mu}}{\text{minimize}} \quad & -\int_0^T \int_{\boldsymbol{\Gamma}} \boldsymbol{f} \cdot \dot{\boldsymbol{x}} \, dS \, dt \\ \text{subject to} \quad & \int_0^T \int_{\boldsymbol{\Gamma}} \boldsymbol{f} \cdot \boldsymbol{e}_1 \, dS \, dt = q \\ & \boldsymbol{U}(\boldsymbol{x}, 0) = \boldsymbol{U}(\boldsymbol{x}, T) \\ & \frac{\partial \boldsymbol{U}}{\partial t} + \nabla \cdot \boldsymbol{F}(\boldsymbol{U}, \nabla \boldsymbol{U}) = 0 \end{aligned}$$

- Isentropic, compressible, Navier-Stokes
- $\mathrm{Re} = 1000$, $\mathrm{M} = 0.2$
- $y(t)$, $\theta(t)$, $c(t)$ parametrized via periodic cubic splines
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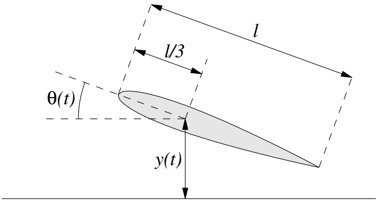


Airfoil schematic, kinematic description

Solution of Time-Periodic, Energetically Optimal Flapping

$$\text{Energy} = 9.4096$$
$$x\text{-impulse} = \text{-}0.1766$$

$$\text{Energy} = 0.45695$$
$$x\text{-impulse} = 0.000$$

Newton-Krylov Shooting Method for Time-Periodic Solutions

- Apply Newton's method to solve nonlinear system of equations

$$\boldsymbol{R}(\boldsymbol{u}_0) = \boldsymbol{u}^{(N_t)}(\boldsymbol{u}_0) - \boldsymbol{u}_0 = 0$$

- Nonlinear iteration defined as

$$\boldsymbol{u}_0 \leftarrow \boldsymbol{u}_0 - \boldsymbol{J}(\boldsymbol{u}_0)^{-1}\boldsymbol{R}(\boldsymbol{u}_0)$$

where $\boldsymbol{J}(\boldsymbol{u}_0) = \dfrac{\partial \boldsymbol{u}^{(N_t)}}{\partial \boldsymbol{u}_0} - \boldsymbol{I}$

- $\dfrac{\partial \boldsymbol{u}^{(N_t)}}{\partial \boldsymbol{u}_0}$ is a **large, dense** matrix and expensive to construct
- Krylov method to solve $\boldsymbol{J}(\boldsymbol{u}_0)^{-1}\boldsymbol{R}(\boldsymbol{u}_0)$ only requires matrix-vector products

$$\boldsymbol{J}(\boldsymbol{u}_0)\boldsymbol{v} = \frac{\partial \boldsymbol{u}^{(N_t)}}{\partial \boldsymbol{u}_0}\boldsymbol{v} - \boldsymbol{v}$$

Fully Discrete Sensitivity Method to Compute $\frac{\partial \boldsymbol{u}^{(N_t)}}{\partial \boldsymbol{u}_0}\boldsymbol{v}$

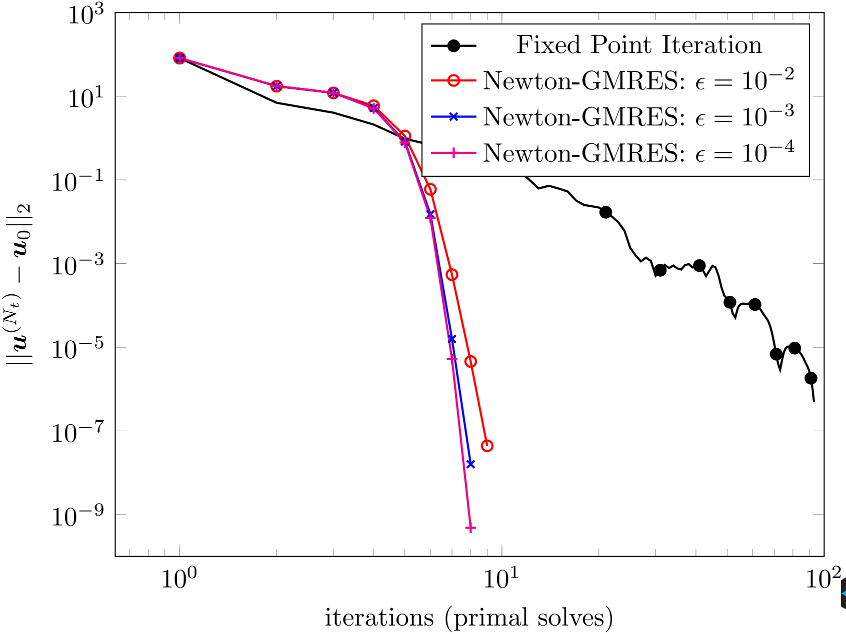
- **Linear** evolution equations solved **forward** in time
- **Primal** state/stage, $\boldsymbol{u}_i^{(n)}$ required at each state/stage of sensitivity problem
- Heavily dependent on **chosen vector**

$$\frac{\partial \boldsymbol{u}^{(0)}}{\boldsymbol{u}_0}\boldsymbol{v} = \boldsymbol{v}$$

$$\frac{\partial \boldsymbol{u}^{(n)}}{\partial \boldsymbol{u}_0}\boldsymbol{v} = \frac{\partial \boldsymbol{u}^{(n-1)}}{\partial \boldsymbol{u}_0}\boldsymbol{v} + \sum_{i=1}^{s} b_i \frac{\partial \boldsymbol{k}_i^{(n)}}{\partial \boldsymbol{u}_0}\boldsymbol{v}$$

$$\mathbb{M}\frac{\partial \boldsymbol{k}_i^{(n)}}{\partial \boldsymbol{u}_0}\boldsymbol{v} = \Delta t_n \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{u}}\left(\boldsymbol{u}_i^{(n)},\ \boldsymbol{\mu},\ t_i^{(n-1)}\right)\left[\frac{\partial \boldsymbol{u}^{(n-1)}}{\partial \boldsymbol{u}_0}\boldsymbol{v} + \sum_{j=1}^{i} a_{ij}\frac{\partial \boldsymbol{k}_j^{(n)}}{\partial \boldsymbol{u}_0}\boldsymbol{v}\right]$$

Newton-GMRES Converges Faster Than Fixed Point Iteration



High-Order Methods To Go Beyond Multiple Choice

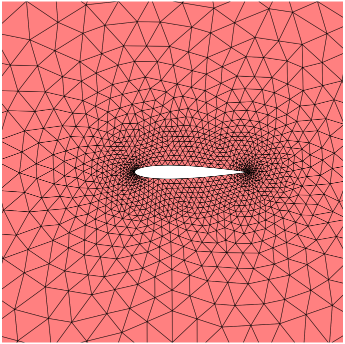
Energy = 9.4096	Energy = 0.45695	Energy = 4.9475
x-impulse = -0.1766	x-impulse = 0.000	x-impulse = -2.500

- Fully discrete **adjoint method for globally high-order discretization** of conservation laws on deforming domains
- Framework, solver, and adjoint-based gradient computation introduced for incorporating **time-periodicity** constraints in optimization

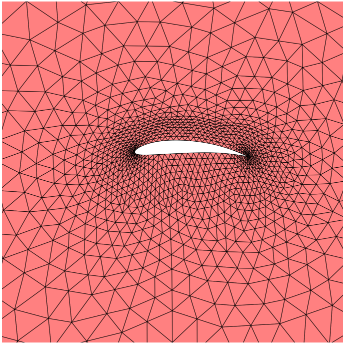
Domain Deformation

- Require mapping $\boldsymbol{x} = \mathcal{G}(\boldsymbol{X}, \boldsymbol{\mu}, t)$ to obtain derivatives $\nabla_{\boldsymbol{X}}\mathcal{G}$, $\frac{\partial}{\partial t}\mathcal{G}$
- Shape deformation, via Radial Basis Functions (RBFs), applied to reference domain

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



Undeformed Mesh

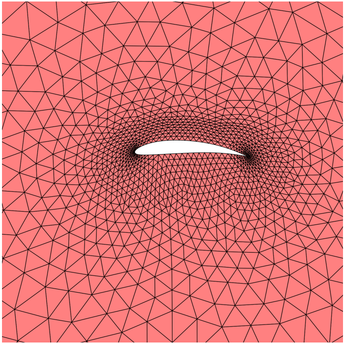


Shape Deformation

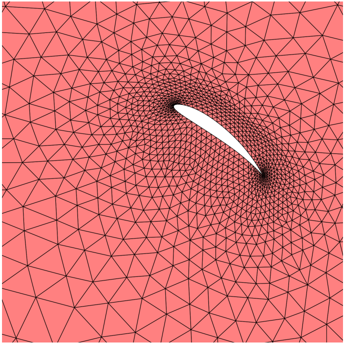
Domain Deformation

- Rigid body translation, $\boldsymbol{v}$, and rotation, $\boldsymbol{Q}$, applied to deformed configuration

$$\boldsymbol{X}'' = \boldsymbol{v} + \boldsymbol{Q}\boldsymbol{X}'$$



Shape Deformation



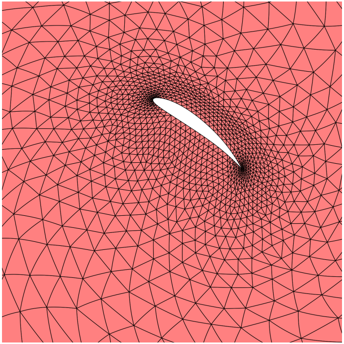
Shape Deformation, Rigid Motion

Domain Deformation

- Spatial blending between deformation with and without rigid body motion to avoid large velocities at far-field

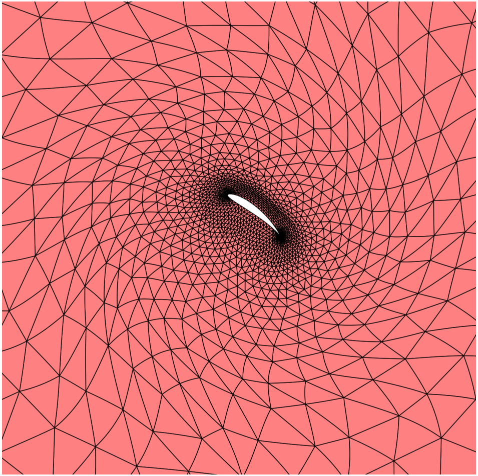
$$\boldsymbol{x} = b(\boldsymbol{X})\boldsymbol{X}' + (1 - b(\boldsymbol{X}))\boldsymbol{X}''$$

  - $b : \mathbb{R}^{n_{sd}} \rightarrow \mathbb{R}$ is a function that smoothly transitions from 0 inside a circle of radius R_1 to 1 outside circle of radius R_2



Blended Mesh

Domain Deformation



Blended Mesh

Arbitrary Lagrangian-Eulerian Description of Conservation Law

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

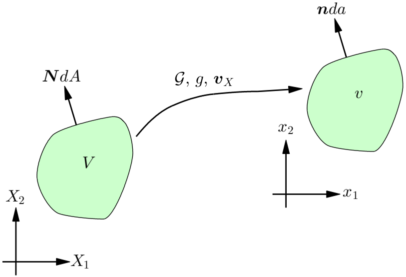
- Introduce transformation

$$\begin{aligned} \boldsymbol{U_X} &= \bar{g}\boldsymbol{U} \\ \boldsymbol{F_X} &= g\boldsymbol{G}^{-1}\boldsymbol{F} - \boldsymbol{U_X}\boldsymbol{G}^{-1}\boldsymbol{v_X} \end{aligned}$$

where

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

$$\frac{\partial \bar{g}}{\partial t} = \nabla_{\boldsymbol{X}} \cdot \left(g\boldsymbol{G}^{-1}\boldsymbol{v_G}\right)$$



- Transformed conservation law[1]

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

[1] Geometric Conservation Law (GCL) satisfied by introduction of $\bar{g}$

Spatial Discretization: Discontinuous Galerkin

- Re-write conservation law as first-order system

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

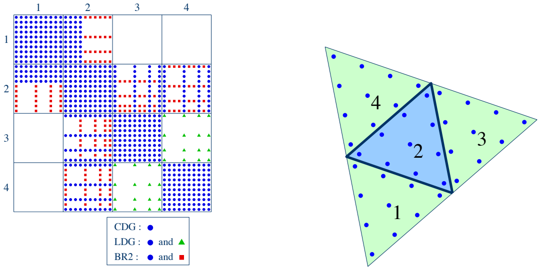
$$\boldsymbol{Q_X} - \nabla_{\boldsymbol{X}} \boldsymbol{U_X} = 0$$

- 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)

$$
\begin{aligned}
\boldsymbol{u}^{(0)} &= \boldsymbol{u}_0(\boldsymbol{\mu}) \\
\boldsymbol{u}^{(n)} &= \boldsymbol{u}^{(n-1)} + \sum_{i=1}^{s} b_i \boldsymbol{k}_i^{(n)} \\
\boldsymbol{u}_i^{(n)} &= \boldsymbol{u}^{(n-1)} + \sum_{j=1}^{i} a_{ij} \boldsymbol{k}_j^{(n)} \\
\mathbb{M}\boldsymbol{k}_i^{(n)} &= \Delta t_n \boldsymbol{r}\left(\boldsymbol{u}_i^{(n)},\ \boldsymbol{\mu},\ t_{n-1} + c_i \Delta t_n\right)
\end{aligned}
$$

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

Butcher Tableau for DIRK scheme

Globally High-Order Discretization

- Fully Discrete Conservation Law

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

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

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

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

- Fully Discrete Output Functional

$$F(\boldsymbol{u}^{(0)}, \dots, \boldsymbol{u}^{(N_t)}, \boldsymbol{k}_1^{(1)}, \dots, \boldsymbol{k}_s^{(N_t)}, \boldsymbol{\mu})$$

Consistent Discretization of Output Quantities

- Consider any quantity of interest of the form

$$\mathcal{F}(\boldsymbol{U}, \boldsymbol{\mu}) = \int_{T_0}^{T_f} \int_{\boldsymbol{\Gamma}} f(\boldsymbol{U}, \boldsymbol{\mu}, t)\, dS\, dt$$

- Define f_h as the high-order approximation of the spatial integral via the DG shape functions

$$f_h(\boldsymbol{u}(t), \boldsymbol{\mu}, t) = \sum_{\mathcal{T}_e \in \mathcal{T}_{\boldsymbol{\Gamma}}} \sum_{\mathcal{Q}_i \in \mathcal{Q}_{\mathcal{T}_e}} w_i f(\boldsymbol{u}_{ei}(t), \boldsymbol{\mu}, t) \approx \int_{\boldsymbol{\Gamma}} f(\boldsymbol{U}, \boldsymbol{\mu}, t)\, dS$$

- Then, the quantity of interest becomes

$$\mathcal{F}(\boldsymbol{U}, \boldsymbol{\mu}) \approx \mathcal{F}_h(\boldsymbol{u}, \boldsymbol{\mu}) = \int_{T_0}^{T_f} f_h(\boldsymbol{u}(t), \boldsymbol{\mu}, t)\, dt$$

Consistent Discretization of Output Quantities

- Semi-discretized output functional

$$\mathcal{F}_h(\boldsymbol{u}, \boldsymbol{\mu}, t) = \int_{T_0}^{t} f_h(\boldsymbol{u}(t), \boldsymbol{\mu}, t)\, dt$$

- Differentiation w.r.t. time leads to the

$$\dot{\mathcal{F}}_h(\boldsymbol{u}, \boldsymbol{\mu}, t) = f_h(\boldsymbol{u}(t), \boldsymbol{\mu}, t)$$

- Write semi-discretized output functional *and* conservation law as monolithic system

$$\begin{bmatrix} \mathbb{M} & \mathbf{0} \\ \mathbf{0} & 1 \end{bmatrix} \begin{bmatrix} \dot{\boldsymbol{u}} \\ \dot{\mathcal{F}}_h \end{bmatrix} = \begin{bmatrix} \boldsymbol{r}(\boldsymbol{u}, \boldsymbol{\mu}, t) \\ f_h(\boldsymbol{u}, \boldsymbol{\mu}, t) \end{bmatrix}$$

- Apply DIRK scheme to obtain

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

$$\mathcal{F}_h^{(n)} = \mathcal{F}_h^{(n-1)} + \sum_{i=1}^{s} b_i f_h\left(\boldsymbol{u}_i^{(n)},\ \boldsymbol{\mu},\ t_i^{(n-1)}\right)$$

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

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

where $t_i^{(n-1)} = t_{n-1} + c_i \Delta t_n$

- Only interested in *final* time

$$F(\boldsymbol{u}^{(n)}, \boldsymbol{k}_i^{(n)}, \boldsymbol{\mu}) = \mathcal{F}_h^{(N_t)}$$

Adjoint Equation Derivation - Outline

- Define **auxiliary** PDE-constrained optimization problem

$$
\begin{aligned}
\underset{\substack{\boldsymbol{u}^{(0)},\ \ldots,\ \boldsymbol{u}^{(N_t)} \in \mathbb{R}^{N_{\boldsymbol{u}}},\\ \boldsymbol{k}_1^{(1)},\ \ldots,\ \boldsymbol{k}_s^{(N_t)} \in \mathbb{R}^{N_{\boldsymbol{u}}}}}{\text{minimize}} \quad & F(\boldsymbol{u}^{(0)},\ \ldots,\ \boldsymbol{u}^{(N_t)},\ \boldsymbol{k}_1^{(1)},\ \ldots,\ \boldsymbol{k}_s^{(N_t)},\ \bar{\boldsymbol{\mu}}) \\
\text{subject to} \quad & \tilde{\boldsymbol{r}}^{(0)} = \boldsymbol{u}^{(0)} - \boldsymbol{u}_0(\bar{\boldsymbol{\mu}}) = 0 \\
& \tilde{\boldsymbol{r}}^{(n)} = \boldsymbol{u}^{(n)} - \boldsymbol{u}^{(n-1)} + \sum_{i=1}^{s} b_i \boldsymbol{k}_i^{(n)} = 0 \\
& \boldsymbol{R}_i^{(n)} = \mathbb{M}\boldsymbol{k}_i^{(n)} - \Delta t_n \boldsymbol{r}\left(\boldsymbol{u}_i^{(n)},\ \bar{\boldsymbol{\mu}},\ t_i^{(n-1)}\right) = 0
\end{aligned}
$$

- Define **Lagrangian**

$$
\mathcal{L}(\boldsymbol{u}^{(n)},\ \boldsymbol{k}_i^{(n)},\ \boldsymbol{\lambda}^{(n)},\ \boldsymbol{\kappa}_i^{(n)}) = F - {\boldsymbol{\lambda}^{(0)}}^T \tilde{\boldsymbol{r}}^{(0)} - \sum_{n=1}^{N_t} {\boldsymbol{\lambda}^{(n)}}^T \tilde{\boldsymbol{r}}^{(n)} - \sum_{n=1}^{N_t} \sum_{i=1}^{s} {\boldsymbol{\kappa}_i^{(n)}}^T \boldsymbol{R}_i^{(n)}
$$

Adjoint Equation Derivation - Outline

- The solution of the optimization problem is given by the **Karush-Kuhn-Tucker (KKT) sytem**

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{u}^{(n)}} = 0, \quad \frac{\partial \mathcal{L}}{\partial \boldsymbol{k}_i^{(n)}} = 0, \quad \frac{\partial \mathcal{L}}{\partial \boldsymbol{\lambda}^{(n)}} = 0, \quad \frac{\partial \mathcal{L}}{\partial \boldsymbol{\kappa}_i^{(n)}} = 0$$

- The derivatives w.r.t. the state variables, $\frac{\partial \mathcal{L}}{\partial \boldsymbol{u}^{(n)}} = 0$ and $\frac{\partial \mathcal{L}}{\partial \boldsymbol{k}_i^{(n)}} = 0$, yield the **fully discrete adjoint equations**

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

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

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

Gradient on Manifold of PDE Solutions 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 $\dfrac{\partial \boldsymbol{k}_i^{(n)}}{\partial \boldsymbol{\mu}}$
- Dependent on *initial condition sensitivity*, $\dfrac{\partial \boldsymbol{u}_0}{\partial \boldsymbol{\mu}}$
  - Compute $\boldsymbol{\lambda}^{(0)}{}^T \dfrac{\partial \boldsymbol{u}_0}{\partial \boldsymbol{\mu}}$ directly if $\boldsymbol{u}_0$ is solution of steady-state equation $\boldsymbol{R}(\boldsymbol{u}_0, \boldsymbol{\mu}) = 0$

$$-\boldsymbol{\lambda}^{(0)}{}^T \frac{\partial \boldsymbol{u}_0}{\partial \boldsymbol{\mu}} = \left[\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{u}}^{-T} \boldsymbol{\lambda}^{(0)} \right]^T \frac{\partial \boldsymbol{R}}{\partial \boldsymbol{\mu}}$$

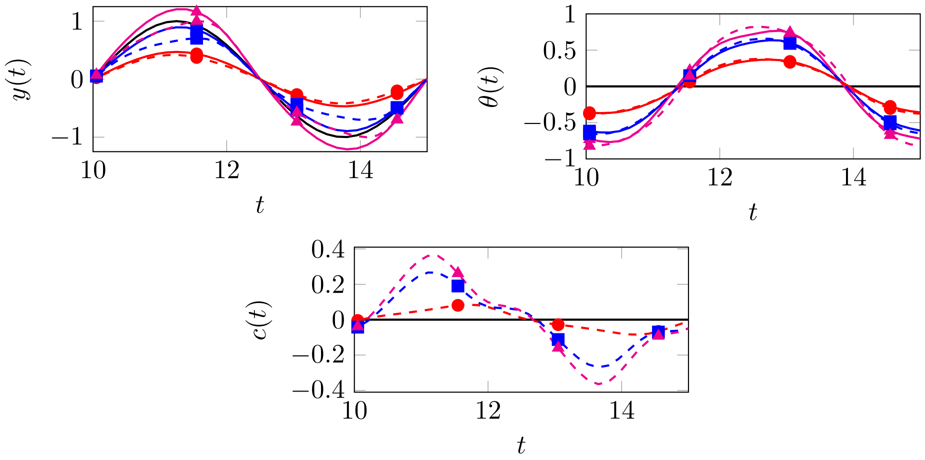
Isentropic, Compressible Navier-Stokes Equations

- Applications in this work focused on compressible Navier-Stokes equations

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) &= 0 \\
\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_i}(\rho u_i u_j + p) &= +\frac{\partial \tau_{ij}}{\partial x_j} \quad \text{for } i = 1, 2, 3 \\
\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_i}\left(u_j(\rho E + p)\right) &= -\frac{\partial q_j}{\partial x_j} + \frac{\partial}{\partial x_j}(u_j \tau_{ij})
\end{aligned}
$$

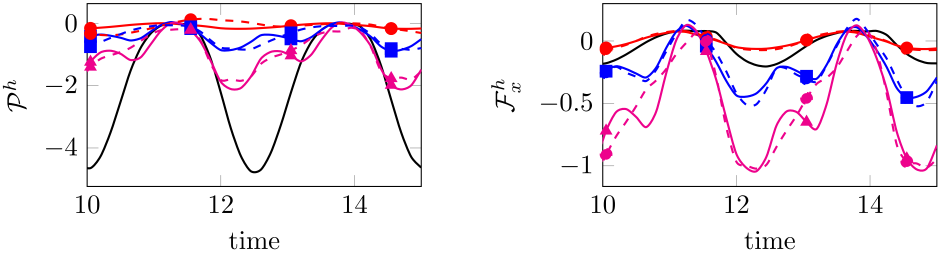
- Isentropic assumption (entropy constant) made to reduce dimension of PDE system from $n_{\text{sd}} + 2$ to $n_{\text{sd}} + 1$

Trajectories of $y(t)$, $\theta(t)$, and $c(t)$



Initial guess ( ), optimal control/fixed shape ($q = 0.0$: , $q = 1.0$: , $q = 2.5$:), and optimal control and time-morphed geometry ($q = 0.0$: , $q = 1.0$: , $q = 2.5$:).

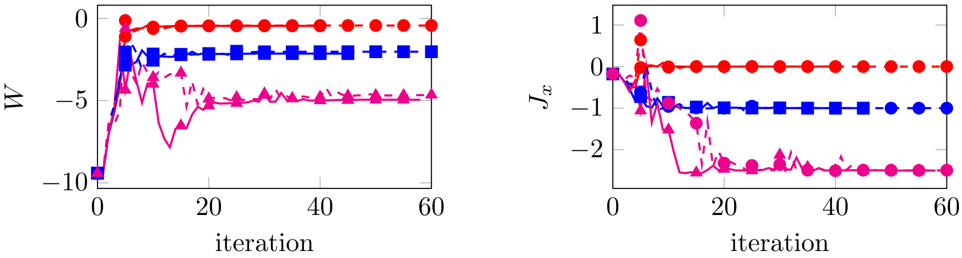
Instantaneous Power ($\mathcal{P}^h$) and x-Force ($\mathcal{F}_x^h$) Exerted on Airfoil



Initial guess (——), optimal control/fixed shape ($q = 0.0$: —●—, $q = 1.0$: —■—, $q = 2.5$: —▲—), and optimal control and time-morphed geometry ($q = 0.0$: - ● -, $q = 1.0$: - ■ -, $q = 2.5$: - ▲ -).

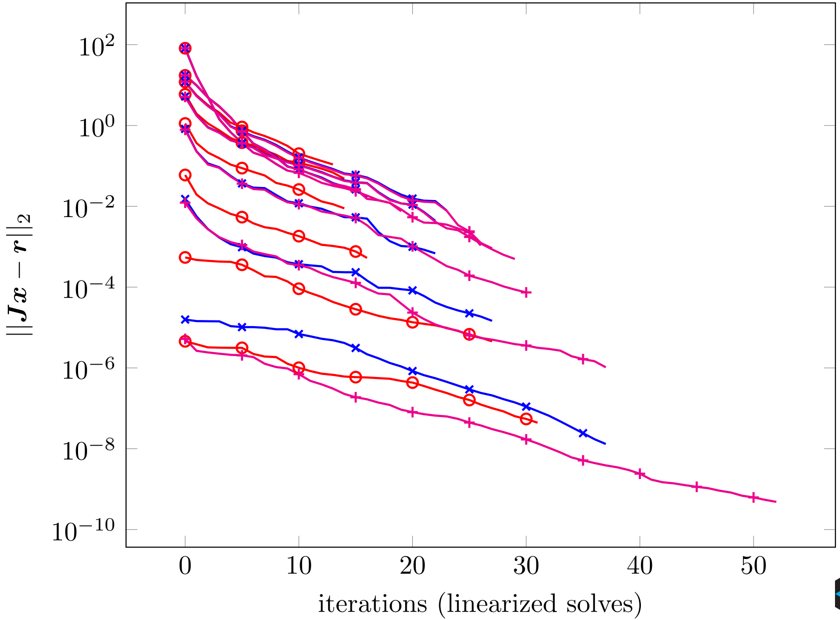
Convergence of Total Work (W) and x-Impulse (J_x) Exerted on Airfoil

Optimization convergence history



Optimal control, fixed shape ($q = 0.0$: , $q = 1.0$: , $q = 2.5$:)
Optimal control, time-morphed geometry ($q = 0.0$: , $q = 1.0$: , $q = 2.5$:)

At the Cost of Linearized Solves



Stability of Periodic Orbits of Fully Discrete PDE

- Let $\boldsymbol{u}_0^*(\boldsymbol{\mu})$ be a fully discrete time-periodic solution of the PDE
- Define the operator

$$\boldsymbol{u}^{(n\cdot N_t)}(\boldsymbol{u}_0;\ \boldsymbol{\mu}) = \boldsymbol{u}^{(N_t)}(\cdot;\ \boldsymbol{\mu}) \circ \cdots \circ \boldsymbol{u}^{(N_t)}(\boldsymbol{u}_0;\ \boldsymbol{\mu})$$

- A Taylor expansion of $\boldsymbol{u}^{(N_t)}$ about the periodic solution leads to

$$\boldsymbol{u}^{(N_t)}(\boldsymbol{u}_0^*(\boldsymbol{\mu});\ \boldsymbol{\mu}) = \boldsymbol{u}_0^*(\boldsymbol{\mu}) + \frac{\partial \boldsymbol{u}^{(N_t)}}{\partial \boldsymbol{u}_0}(\boldsymbol{u}_0^*(\boldsymbol{\mu});\ \boldsymbol{\mu}) \cdot \Delta \boldsymbol{u} + \mathcal{O}(||\Delta \boldsymbol{u}||^2)$$

  where time-periodicity of $\boldsymbol{u}_0^*(\boldsymbol{\mu})$ was used
- Repeated application of leads to

$$\boldsymbol{u}^{(n\cdot N_t)}(\boldsymbol{u}_0^*(\boldsymbol{\mu}) + \Delta \boldsymbol{u};\ \boldsymbol{\mu}) = \boldsymbol{u}_0^*(\boldsymbol{\mu}) + \left[\frac{\partial \boldsymbol{u}^{(N_t)}}{\partial \boldsymbol{u}_0}(\boldsymbol{u}_0^*(\boldsymbol{\mu});\ \boldsymbol{\mu})\right]^n \Delta \boldsymbol{u} + \mathcal{O}(||\Delta \boldsymbol{u}||^{n+1})$$

- Periodic orbit is stable if eigenvalues of $\dfrac{\partial \boldsymbol{u}^{(N_t)}}{\partial \boldsymbol{u}_0}(\boldsymbol{u}_0^*(\boldsymbol{\mu});\ \boldsymbol{\mu})$ have magnitude less than unity

Conclusion

- Derived adjoint equations for DG-DIRK discretization of general conservation laws on deforming domain
- Introduced fully discrete adjoint method for computing gradients of quantities of interest
  - Framework demonstrated on the computation of energetically optimal motions of a 2D airfoil in a flow field with constraints
- Introduced fully discrete sensitivity equations and used Newton-Krylov shooting method to compute time-periodic flows
- Framework and solver introduced for incorporating time-periodicity constraints in optimization problem
- **Next steps**: 3D, multiphysics, model reduction