

# Integrated computational physics and numerical optimization

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Optimize physics

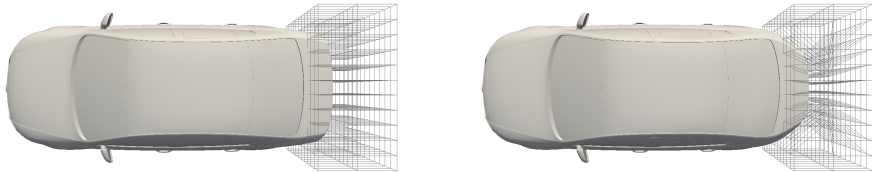
Optimize numerics

Optimize physics

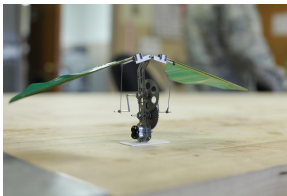
Optimize numerics

# PDE optimization is ubiquitous in science and engineering

**Design:** Find system that optimizes performance metric, satisfies constraints



Aerodynamic shape design of automobile

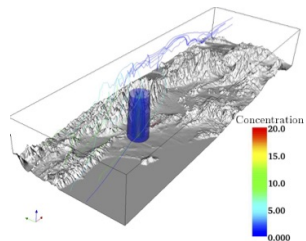
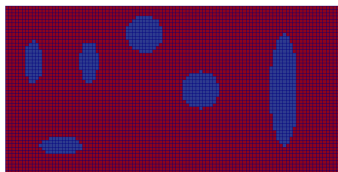


Optimal flapping motion of micro aerial vehicle

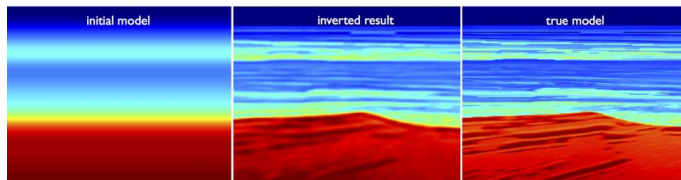


# PDE optimization is ubiquitous in science and engineering

**Inverse problems:** Infer the problem setup given solution observations



Material inversion: find inclusions from acoustic, structural measurements  
Source inversion: find source of contaminant from downstream measurements



Full waveform inversion: estimate subsurface of crust from acoustic measurements

# Unsteady PDE-constrained optimization formulation

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

$$\underset{\mathbf{U}, \boldsymbol{\mu}}{\text{minimize}} \quad \mathcal{J}(\mathbf{U}, \boldsymbol{\mu})$$

$$\text{subject to} \quad \mathbf{C}(\mathbf{U}, \boldsymbol{\mu}) \leq 0$$

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{U}, \nabla \mathbf{U}) = 0 \quad \text{in } v(\boldsymbol{\mu}, t)$$

$\mathbf{U}(\mathbf{x}, t)$

PDE solution

$\boldsymbol{\mu}$

design/control parameters

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

objective function

$$\mathbf{C}(\mathbf{U}, \boldsymbol{\mu}) = \int_{T_0}^{T_f} \int_{\Gamma} \mathbf{c}(\mathbf{U}, \boldsymbol{\mu}, t) dS dt$$

constraints

# Nested approach to PDE-constrained optimization

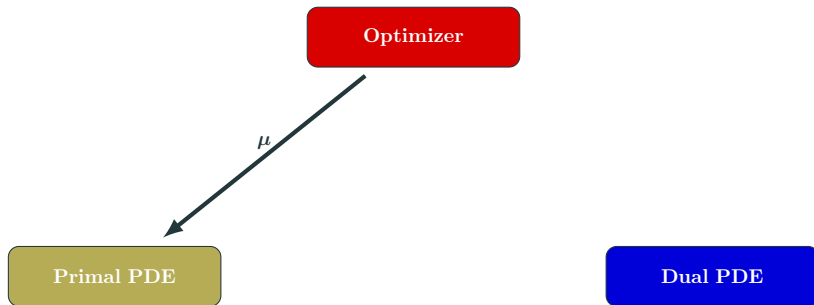
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graph TD; Optimizer[Optimizer]; PrimalPDE[Primal PDE]; DualPDE[Dual PDE]; Optimizer --- PrimalPDE; Optimizer --- DualPDE;
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Optimizer

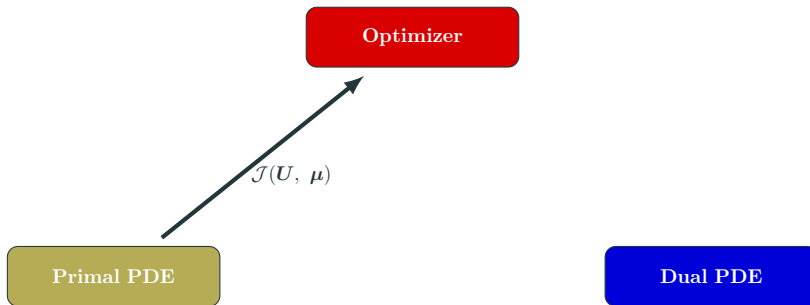
Primal PDE

Dual PDE

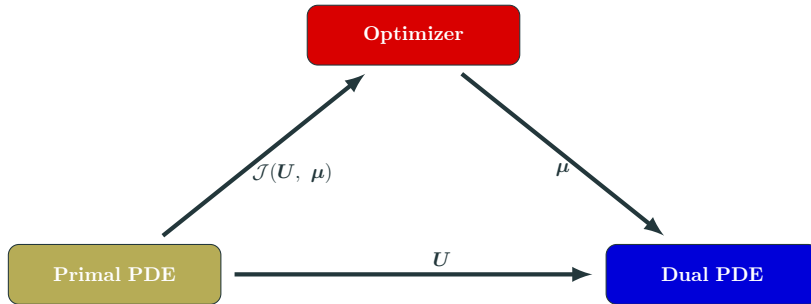
# Nested approach to PDE-constrained optimization



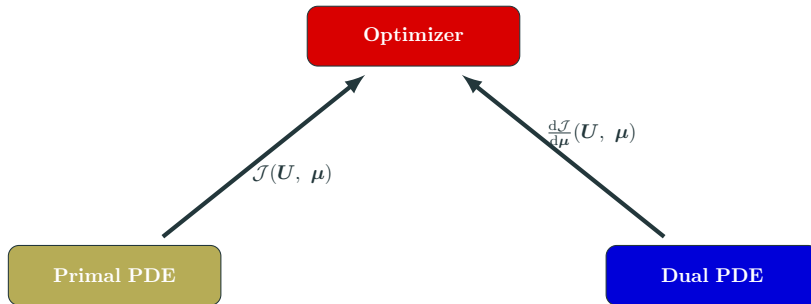
# Nested approach to PDE-constrained optimization



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# Nested approach to PDE-constrained optimization



# 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  $V$

$$\frac{\partial \mathbf{U}_X}{\partial t} \Big|_{\mathbf{X}} + \nabla_{\mathbf{X}} \cdot \mathbf{F}_X(\mathbf{U}_X, \nabla_{\mathbf{X}} \mathbf{U}_X) = 0$$

**Space discretization:** discontinuous Galerkin

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

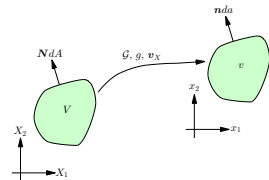
**Time discretization:** diagonally implicit RK

$$\mathbf{u}_n = \mathbf{u}_{n-1} + \sum_{i=1}^s b_i \mathbf{k}_{n,i}$$

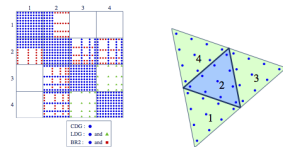
$$\mathbf{M} \mathbf{k}_{n,i} = \Delta t_n \mathbf{r}(\mathbf{u}_{n,i}, \boldsymbol{\mu}, t_{n,i})$$

**Quantity of interest:** solver-consistency

$$F(\mathbf{u}_0, \dots, \mathbf{u}_{N_t}, \mathbf{k}_{1,1}, \dots, \mathbf{k}_{N_t,s}, \boldsymbol{\mu})$$



Mapping-Based ALE



DG Discretization

$c_1$	$a_{11}$			
$c_2$	$a_{21}$	$a_{22}$		
$\vdots$	$\vdots$	$\vdots$	$\ddots$	
$c_s$	$a_{s1}$	$a_{s2}$	$\cdots$	$a_{ss}$
	$b_1$	$b_2$	$\cdots$	$b_s$

Butcher Tableau for DIRK



# Adjoint method to efficiently compute gradients of QoI

*Fully discrete* output function i.e., either **objective** or a **constraint**

$$F(\boldsymbol{\mu}) = F(\mathbf{u}_0, \dots, \mathbf{u}_n, \mathbf{k}_{1,1}, \dots, \mathbf{k}_{N_t,s}, \boldsymbol{\mu})$$

# Adjoint method to efficiently compute gradients of QoI

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$$F(\boldsymbol{\mu}) = F(\mathbf{u}_0, \dots, \mathbf{u}_n, \mathbf{k}_{1,1}, \dots, \mathbf{k}_{N_t,s}, \boldsymbol{\mu})$$

*Total derivative* with respect to parameters  $\boldsymbol{\mu}$

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

However, the sensitivities,  $\frac{\partial \mathbf{u}_n}{\partial \boldsymbol{\mu}}$  and  $\frac{\partial \mathbf{k}_{n,i}}{\partial \boldsymbol{\mu}}$ , are expensive to compute, requiring the solution of  $n_{\boldsymbol{\mu}}$  linear evolution equations

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## Adjoint method

Alternative method for computing  $DF$  that does not require sensitivities

# Dissection of fully discrete adjoint equations

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

$$\begin{aligned}\lambda_{N_t} &= \frac{\partial F}{\partial \mathbf{u}_{N_t}}^T \\ \lambda_{n-1} &= \lambda_n + \frac{\partial F}{\partial \mathbf{u}_{n-1}}^T + \sum_{i=1}^s \Delta t_n \frac{\partial \mathbf{r}}{\partial \mathbf{u}}(\mathbf{u}_{n,i}, \boldsymbol{\mu}, t_{n-1} + c_i \Delta t_n)^T \boldsymbol{\kappa}_{n,i} \\ M^T \boldsymbol{\kappa}_{n,i} &= \frac{\partial F}{\partial \mathbf{u}_{N_t}}^T + b_i \lambda_n + \sum_{j=i}^s a_{ji} \Delta t_n \frac{\partial \mathbf{r}}{\partial \mathbf{u}}(\mathbf{u}_{n,j}, \boldsymbol{\mu}, t_{n-1} + c_j \Delta t_n)^T \boldsymbol{\kappa}_{n,j}\end{aligned}$$

Gradient reconstruction via dual variables

$$DF = \frac{\partial F}{\partial \boldsymbol{\mu}} + \lambda_0^T \frac{\partial g}{\partial \boldsymbol{\mu}}(\boldsymbol{\mu}) + \sum_{n=1}^{N_t} \Delta t_n \sum_{i=1}^s \boldsymbol{\kappa}_{n,i}^T \frac{\partial \mathbf{r}}{\partial \boldsymbol{\mu}}(\mathbf{u}_{n,i}, \boldsymbol{\mu}, t_{n,i})$$

[Zahr and Persson, 2016]

# Optimal rigid body motion (RBM), time-morph geometry (TMG)

Energy = 9.4096

Thrust = 0.1766

Energy = 4.9476

Thrust = 2.500

Energy = 4.6182

Thrust = 2.500

Initial Guess

Optimal RBM

$T_x = 2.5$

Optimal RBM/TMG

$T_x = 2.5$

# Energetically optimal flapping in three dimensions

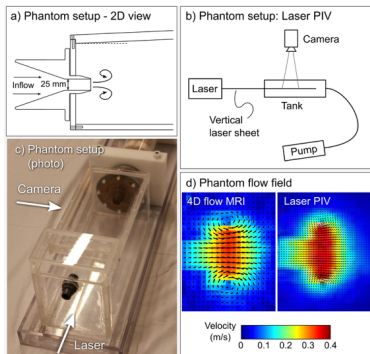
Energy = 1.4459e-01

Thrust = -1.1192e-01

Energy = 3.1378e-01

Thrust = 0.0000e+00

# Super-resolution MR images through optimization



Experimental setup

Noisy, low-resolution MRI data

**Goal:** visualize *in vivo* flow with high-resolution and accurately compute clinically relevant quantities from quick scans

**Idea:** determine CFD parameters (material properties, boundary conditions) such that the simulation matches MRI data using optimization

# MRI optimization formulation that respects scanner physics

$$\underset{\boldsymbol{\mu}}{\text{minimize}} \quad \sum_{i=1}^{n_{xyz}} \sum_{n=1}^{n_t} \frac{\alpha_{i,n}}{2} \left\| \mathbf{d}_{i,n}(\mathbf{U}(\boldsymbol{\mu}), \boldsymbol{\mu}) - \mathbf{d}_{i,n}^* \right\|_2^2$$

$\mathbf{d}_{i,n}^*$  : MRI measurement taken in voxel  $i$  at the  $n$ th time sample

$\mathbf{d}_{i,n}(\mathbf{U}, \boldsymbol{\mu})$ : computational representation of  $\mathbf{d}_{i,n}^*$



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$$\mathbf{d}_{i,n}(\mathbf{U}, \boldsymbol{\mu}) = \int_0^T \int_V w_{i,n}(\mathbf{x}, t) \cdot \mathbf{U}(\mathbf{x}, t) dV dt$$

$$w_{i,n}(\mathbf{x}, t) = \chi_s(\mathbf{x}; \mathbf{x}_i, \Delta\mathbf{x}) \chi_t(t; t_n, \Delta t)$$

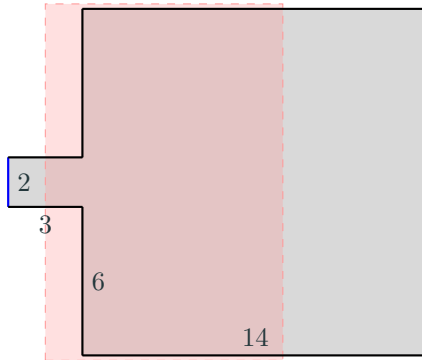
$$\chi_t(s; c, w) = \frac{1}{1 + e^{-(s-(c-0.5w))/\sigma)}} - \frac{1}{1 + e^{-(s-(c+0.5w))/\sigma}}$$

$$\chi_s(\mathbf{x}; \mathbf{c}, \mathbf{w}) = \chi_t(x_1; c_1, w_1) \chi_t(x_2; c_2, w_2) \chi_t(x_3; c_3, w_3)$$

$\mathbf{x}_i$  center of  $i$ th MRI voxel,  $\Delta\mathbf{x}$  size of MRI voxel

$t_n$  time instance of  $n$ th MRI sample,  $\Delta t$  sampling interval in time

# Model problem with synthetic data



Viscous wall (—), parametrized inflow (—), and outflow (—).

MRI data collected in the red shaded region.

High-quality reconstruction from coarse MRI grid (space:  $24 \times 36$ , time: 10) and low noise (3%)

Reconstructed flow

Synthetic MRI data  $\mathbf{d}_{i,n}^*$  (top) and  
computational representation of MRI  
data  $\mathbf{d}_{i,n}$  (bottom)

# High-quality reconstruction from fine MRI grid (space: $40 \times 60$ , time: 20) and high noise (10%)

Reconstructed flow

Synthetic MRI data  $\mathbf{d}_{i,n}^*$  (top) and  
computational representation of MRI  
data  $\mathbf{d}_{i,n}$  (bottom)

# High-quality reconstruction with experimental data: pulsatile flow

CFD-based reconstruction from quick, low-resolution scan matches laser PIV measurements better than slow, high-resolution scan

MRI data

Reconstructed flow

## Extension: Parametrized time domain [Wang et al., 2017]

Parametrization of time domain, e.g., flapping frequency, leads to parametrization of time discretization in fully discrete setting

$$T(\boldsymbol{\mu}) = N_t \Delta t \implies N_t = N_t(\boldsymbol{\mu}) \text{ or } \Delta t = \Delta t(\boldsymbol{\mu})$$

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Does not change adjoint equations themselves, only reconstruction of gradient from adjoint solution



## Energetically optimal flapping vs. required thrust

Energy = 1.8445  
Thrust = 0.06729

Energy = 0.21934  
Thrust = 0.0000

Energy = 6.2869  
Thrust = 2.5000

Initial Guess

Optimal  
 $T_x = 0$

Optimal  
 $T_x = 2.5$

## Extension: Multiphysics problems [Huang et al., 2018]

For problems that involve the interaction of multiple types of physical phenomena, *no changes required* if monolithic system considered

$$\mathbf{M}_0 \dot{\mathbf{u}}_0 = \mathbf{r}_0(\mathbf{u}_0, \mathbf{c}_0(\mathbf{u}_0, \mathbf{u}_1))$$

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Adjoint equations inherit **explicit-implicit** structure

# High-order method for general multiphysics problems with unconditional linear stability

Particle-laden flow

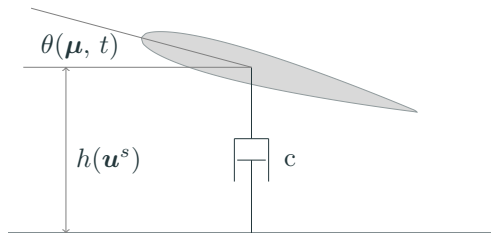
Fluid-structure interaction

# Optimal energy harvesting from foil-damper system

**Goal:** Maximize energy harvested from foil-damper system

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

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



$$\mu_1^* \approx 45^\circ$$

# High-order methods for PDE-constrained optimization

- Developed **fully discrete adjoint method** for **high-order** numerical discretizations of PDEs and QoIs
- Used to compute **gradients** of QoI for use in gradient-based numerical optimization method
- Treatment of **parametrized time domain** (optimal frequency)
- Explicit enforcement of **time-periodicity constraints**
- Extension to **multiphysics** (fluid-structure interaction, particle-laden flow, ...)
- **Applications:** optimal flapping flight, energy harvesting, data assimilation

# Integrating computational physics and numerical optimization

Optimize physics

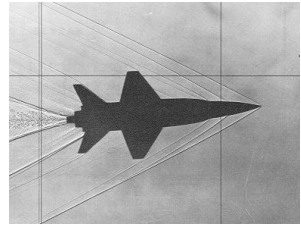
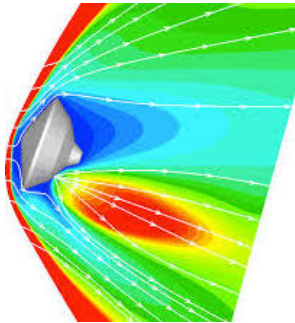
Optimize numerics



# Discontinuities often arise in engineering systems, particularly in those involving compressible flows: shock waves, contact lines

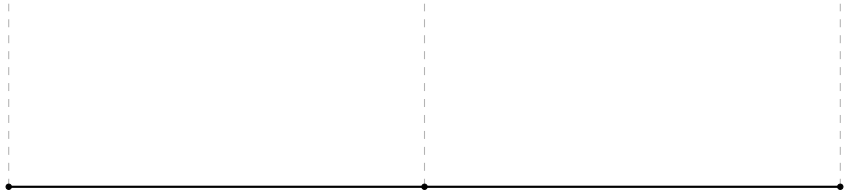
Supersonic and transonic flow around commercial planes and fighter jets

Hypersonics, e.g., re-entry of vehicles in atmosphere, and scramjets



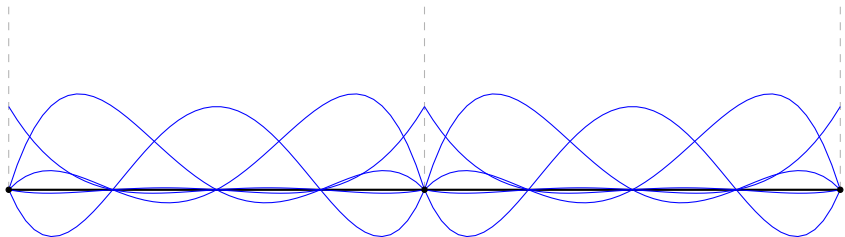
Other applications with discontinuities: fracture, problems with interfaces

# State-of-the-art numerical methods for resolving shocks



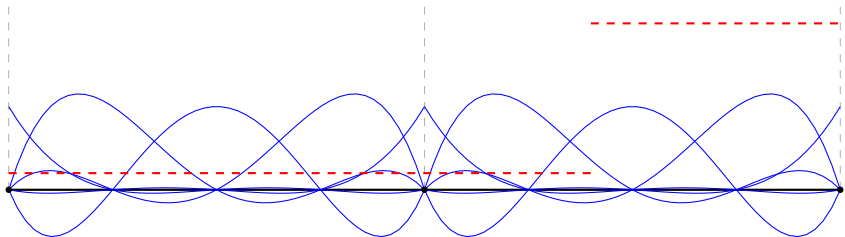
Fundamental issue: approximate discontinuity with polynomial basis

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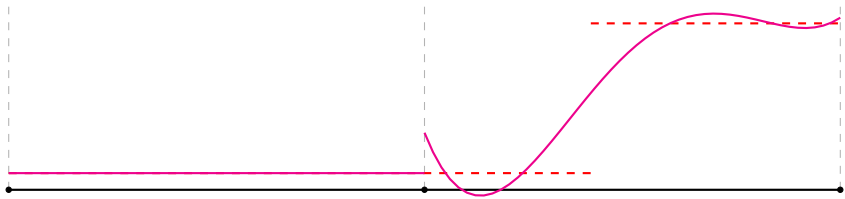
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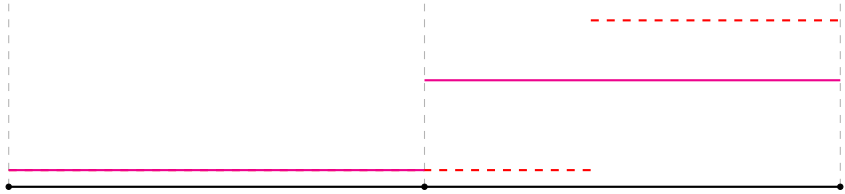
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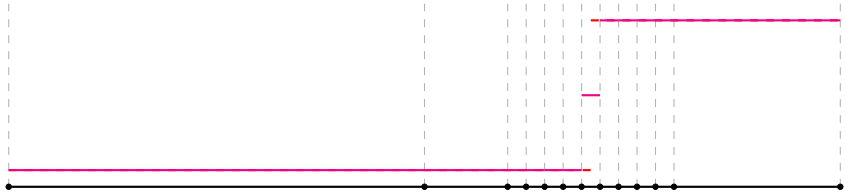


Fundamental issue: approximate discontinuity with polynomial basis

Existing solutions: **limiting**, artificial viscosity

Drawbacks: order reduction, local refinement

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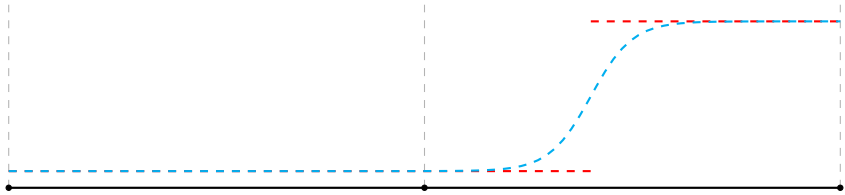


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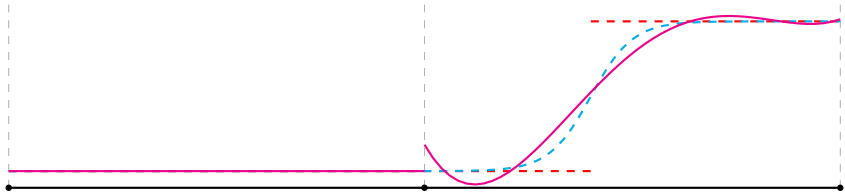
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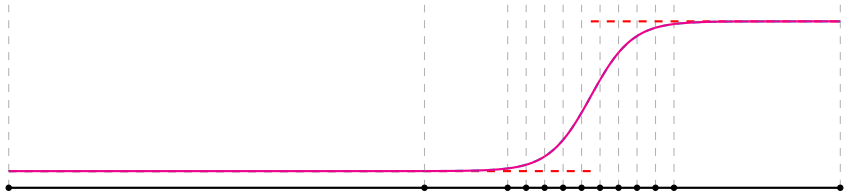


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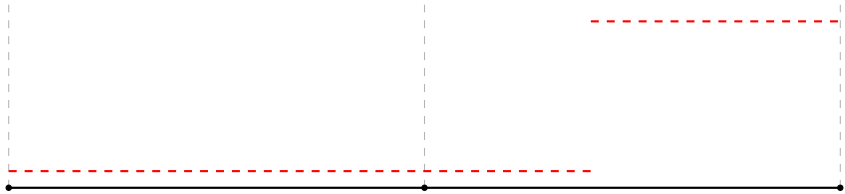


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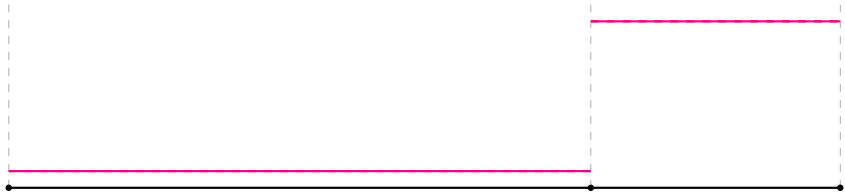
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Proposed solution: align features of solution basis with features in the solution using optimization formulation and solver

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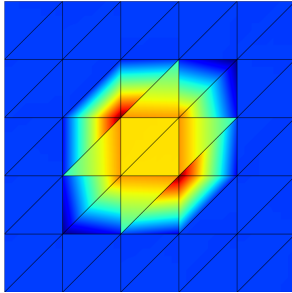
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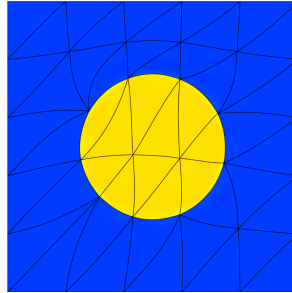
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# Tracking method for stable, high-order resolution of discontinuities

Goal: Align element faces with (unknown) discontinuities to perfectly capture them and approximate smooth regions to high-order



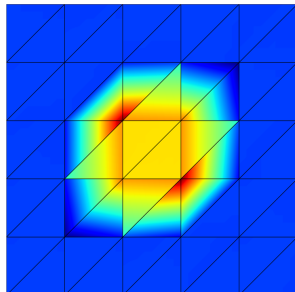
Non-aligned



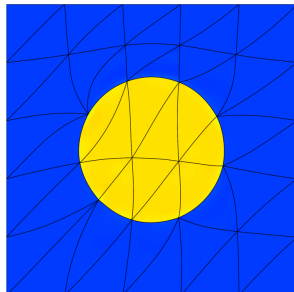
Discontinuity-aligned

# Tracking method for stable, high-order resolution of discontinuities

Goal: Align element faces with (unknown) discontinuities to perfectly capture them and approximate smooth regions to high-order



Non-aligned



Discontinuity-aligned

## Ingredients

- Discontinuous Galerkin discretization: inter-element jumps, high-order
- Optimization formulation that penalizes local instabilities in the solution and enforces the discrete PDE
- Full space solver that converges the solution and mesh simultaneously to ensure solution of PDE never required on non-aligned mesh

# Discontinuity-tracking as PDE-constrained optimization problem

$$\begin{aligned} & \underset{\mathbf{u}, \mathbf{x}}{\text{minimize}} && f(\mathbf{u}, \mathbf{x}) \\ & \text{subject to} && \mathbf{r}(\mathbf{u}, \mathbf{x}) = 0 \end{aligned}$$

$$\begin{aligned} & \underset{\mathbf{u}, \mathbf{x}}{\text{minimize}} && f(\mathbf{u}, \mathbf{x}) \\ & \text{subject to} && \mathbf{r}(\mathbf{u}, \mathbf{x}) = 0 \end{aligned}$$

## Objective function

Must **obtain minimum** when mesh face aligned with shock and **monotonically** decreases to minimum in neighborhood of radius  $\mathcal{O}(h/2)$  about discontinuity



# Discontinuity-tracking as PDE-constrained optimization problem

$$\begin{aligned} & \underset{\mathbf{u}, \mathbf{x}}{\text{minimize}} && f(\mathbf{u}, \mathbf{x}) \\ & \text{subject to} && \mathbf{r}(\mathbf{u}, \mathbf{x}) = 0 \end{aligned}$$

## Objective function

Must **obtain minimum** when mesh face aligned with shock and **monotonically** decreases to minimum in neighborhood of radius  $\mathcal{O}(h/2)$  about discontinuity

## Optimization approach

Cannot use **nested** approach where constraint  $\mathbf{r}(\mathbf{u}, \mathbf{x}) = 0$  is eliminated because discrete PDE cannot be solved unless  $\mathbf{x} = \mathbf{x}^* \implies$  **full space** approach required

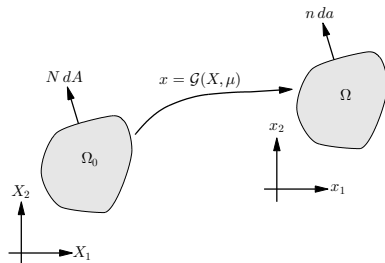
# Transformed conservation law from deformation of physical domain

Consider physical domain as the result of a  $\mu$ -parametrized diffeomorphism applied to some reference domain  $\Omega_0$

$$\Omega = \mathcal{G}(\Omega_0, \mu)$$

Re-write conservation law on reference domain

$$\begin{aligned} \nabla \cdot \mathcal{F}(U) = 0 \quad \text{in } \mathcal{G}(\Omega_0, \mu) &\implies \nabla_X \cdot F(u, \mu) = 0 \quad \text{in } \Omega_0, \\ u = g_\mu U, \quad F(u, \mu) = g_\mu \mathcal{F}(g_\mu^{-1} u) G_\mu^{-T}, \quad G_\mu = \frac{\partial}{\partial X} \mathcal{G}(X, \mu), \quad g_\mu = \det G_\mu \end{aligned}$$



Mapping between reference and physical domains

# Discontinuous Galerkin discretization of conservation law

Element-wise weak form of transformed conservation law

$$\int_{\partial K} \psi \cdot F(u, \mu) N dA - \int_K F(u, \mu) : \nabla_X \psi dV = 0$$

Global weak form and introduction of numerical flux

$$\sum_{K \in \mathcal{E}_{h,p}} \int_{\partial K} \psi \cdot F^*(u, \mu, N) dA - \int_{\Omega_0} F(u, \mu) : \nabla_X \psi dV = 0$$

Strict requirements on numerical flux since inter-element jumps will not tend to zero on shock surface



Fully discrete transformed conservation law in terms of the discrete state vector  $\mathbf{u}$  and coordinates of physical mesh  $\mathbf{x}$

$$\mathbf{r}(\mathbf{u}, \mathbf{x}) = 0$$

## Objective function: penalize oscillations and mesh distortion

Consider a discontinuity indicator that aims to penalize oscillations in finite-dimensional solution

$$f_{shk}(\mathbf{u}, \mathbf{x}) = h_0^{-2} \sum_{K \in \mathcal{E}_{h,p}} \int_{\mathcal{G}(K, \mathbf{x})} \|u_{h,p} - \bar{u}_{h,p}^K\|_{\mathbf{W}}^2 dV,$$

$$\bar{u}_{h,p}^K = \frac{1}{|\mathcal{G}(K, \mathbf{x})|} \int_{\mathcal{G}(K, \mathbf{x})} u_{h,p} dV, \quad |\mathcal{G}(K, \mathbf{x})| = \int_{\mathcal{G}(K, \mathbf{x})} dV, \quad h_0 = |\Omega_0|^{1/d}$$

## Objective function: penalize oscillations and mesh distortion

Consider a discontinuity indicator that aims to penalize oscillations in finite-dimensional solution

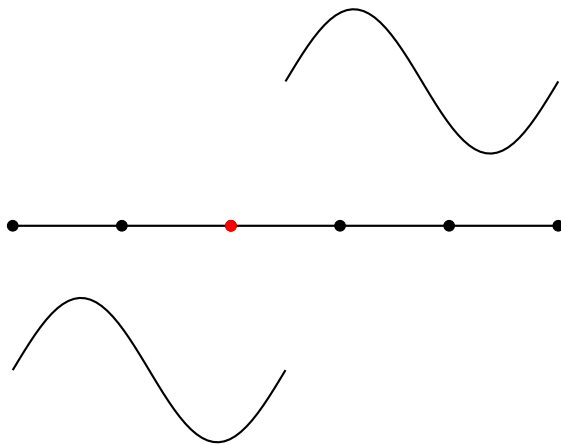
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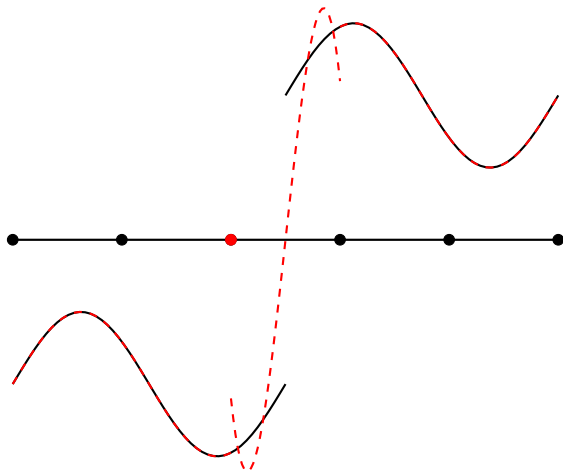
Construct objective function as weighted combination between discontinuity indicator and mesh distortion metric

$$f(\mathbf{u}, \mathbf{x}; \alpha) = f_{shk}(\mathbf{u}, \mathbf{x}) + \alpha f_{msh}(\mathbf{x})$$

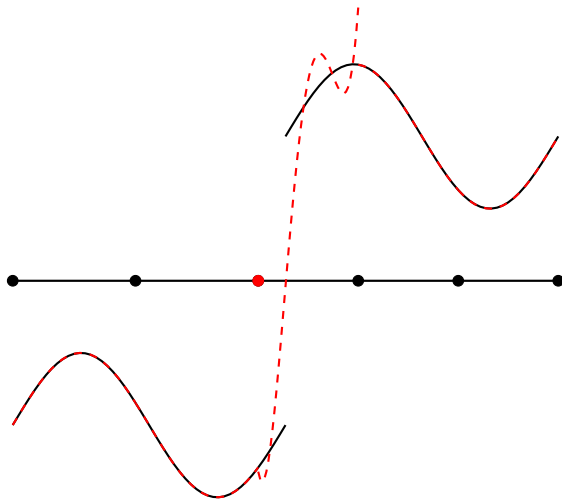
# One-dimensional mesh parametrization and objective function test



# One-dimensional mesh parametrization and objective function test

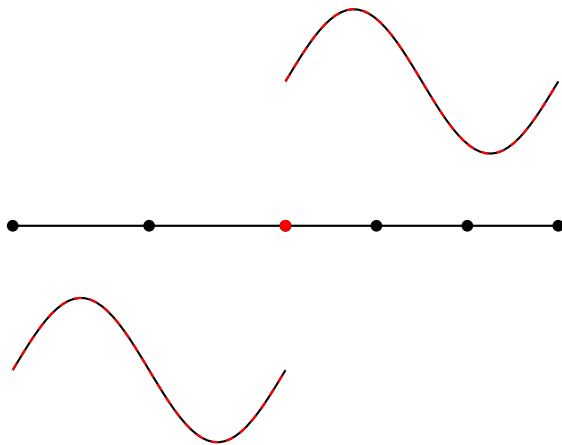


# One-dimensional mesh parametrization and objective function test

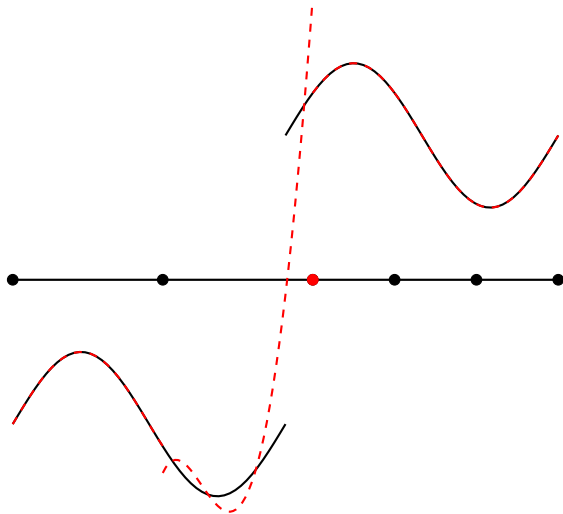




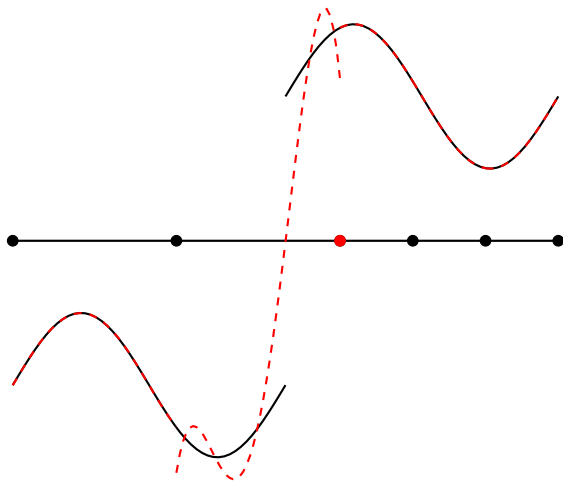
# One-dimensional mesh parametrization and objective function test



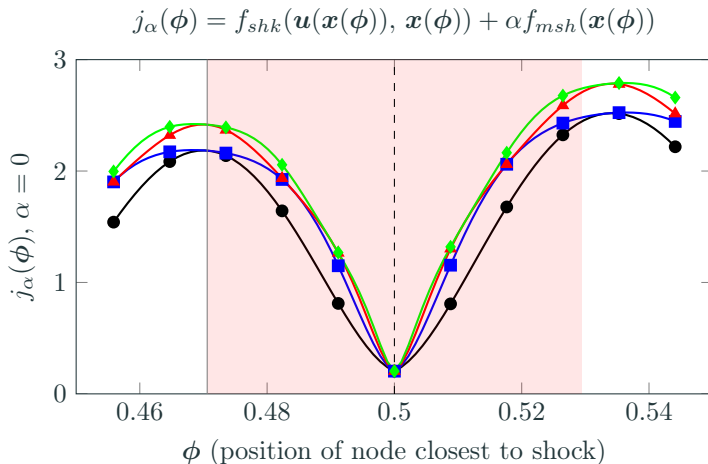
# One-dimensional mesh parametrization and objective function test



# One-dimensional mesh parametrization and objective function test



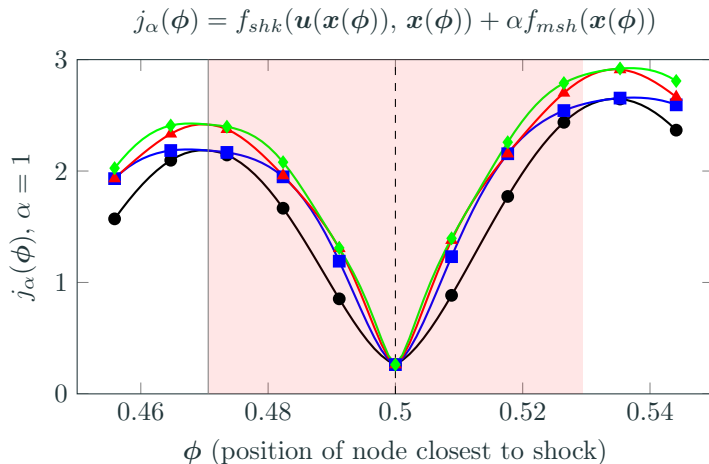
# Objective function monotonically approaches minimum as mesh aligns with discontinuity, regardless of $p$ , for a range of $\alpha$



Objective function as an element face is smoothly swept across discontinuity (---):

$p = 1$  (—●—),  $p = 2$  (—■—),  $p = 3$  (—▲—),  $p = 4$  (—◆—).

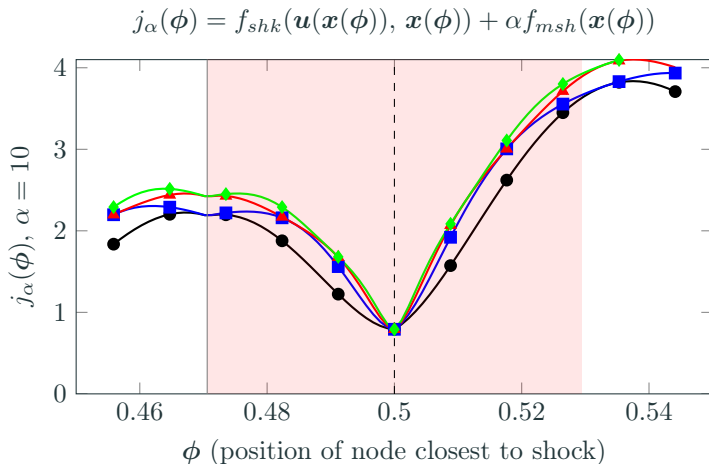
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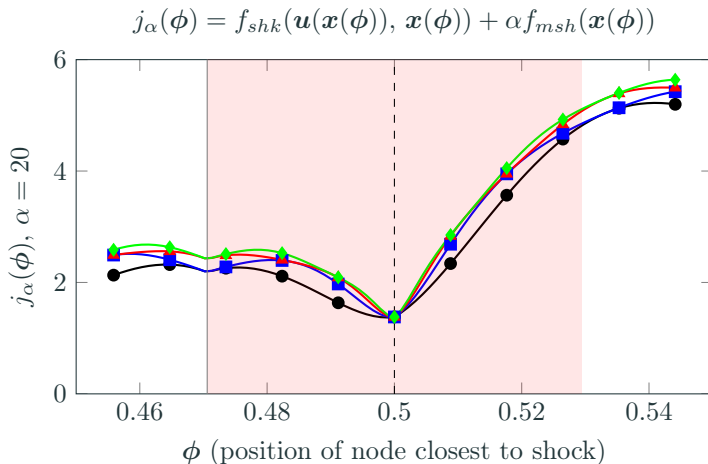
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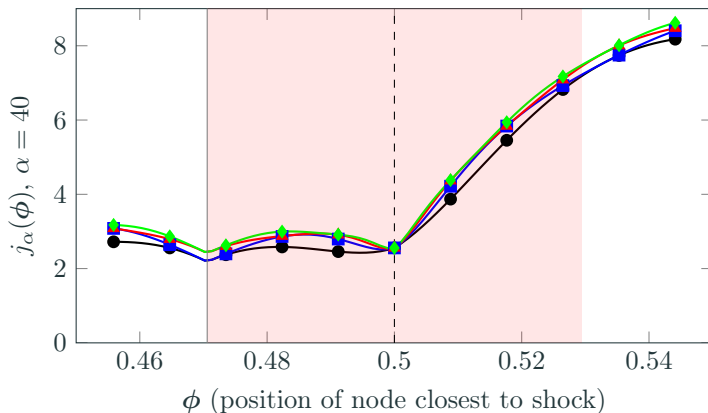


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# Objective function monotonically approaches minimum as mesh aligns with discontinuity, regardless of $p$ , for a range of $\alpha$

$$j_\alpha(\phi) = f_{shk}(\mathbf{u}(\mathbf{x}(\phi)), \mathbf{x}(\phi)) + \alpha f_{msh}(\mathbf{x}(\phi))$$

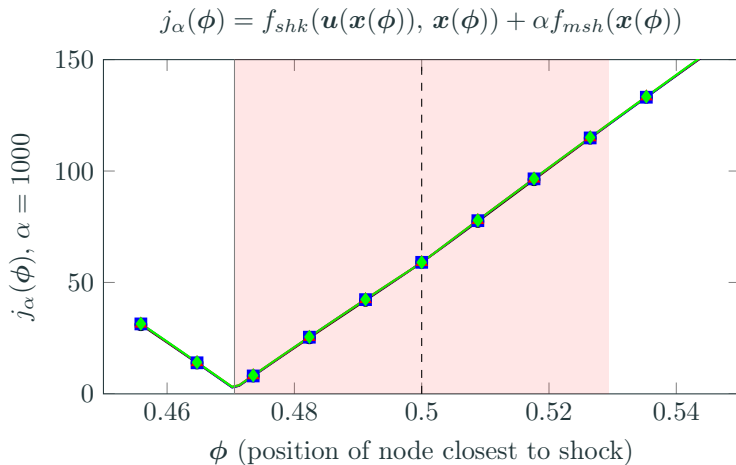


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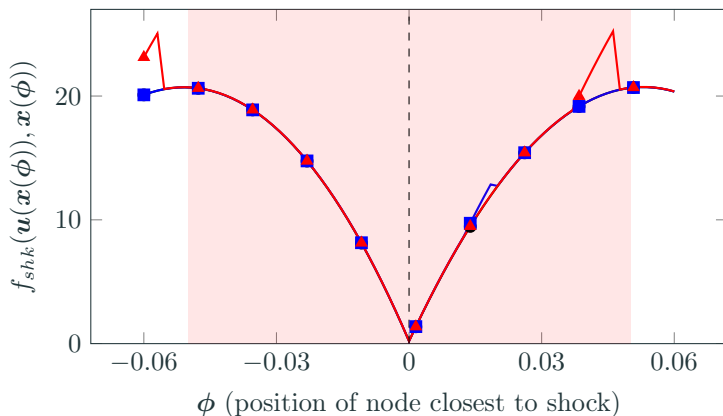
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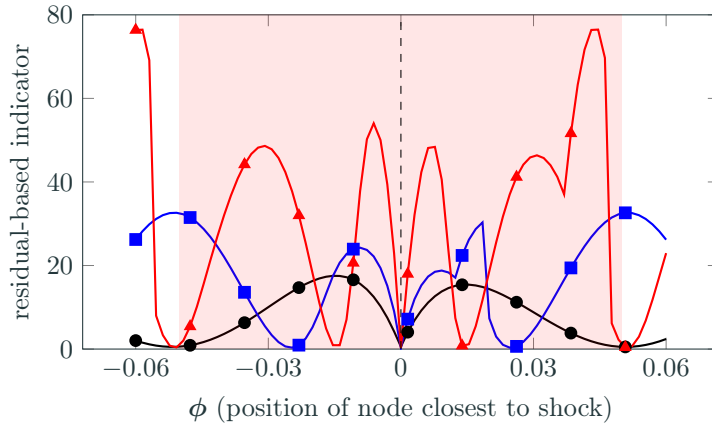
Proposed discontinuity indicator is monotonic and attains minimum at discontinuity, whereas other indicators are not monotonic



Objective function as an element face is smoothly swept across discontinuity (---):

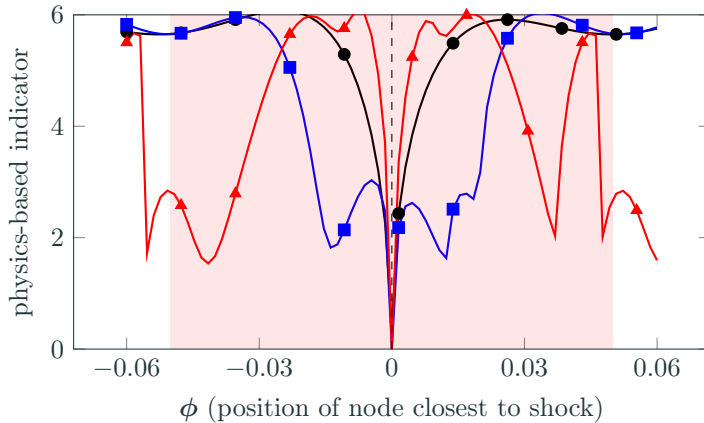
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Objective function as an element face is smoothly swept across discontinuity (---):  
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Cannot use **nested approach** to PDE optimization because it requires solving  $r(u, x) = 0$  for  $x \neq x^* \implies$  **crash**

**Full space approach:**  $u \rightarrow u^*$  and  $x \rightarrow x^*$  *simultaneously*

---

<sup>1</sup>usually requires globalization such as linesearch or trust-region

Cannot use **nested approach** to PDE optimization because it requires solving  $r(\mathbf{u}, \mathbf{x}) = 0$  for  $\mathbf{x} \neq \mathbf{x}^* \implies$  **crash**

**Full space approach:**  $\mathbf{u} \rightarrow \mathbf{u}^*$  and  $\mathbf{x} \rightarrow \mathbf{x}^*$  *simultaneously*

Define Lagrangian

$$\mathcal{L}(\mathbf{u}, \mathbf{x}, \boldsymbol{\lambda}) = f(\mathbf{u}; \mathbf{x}) - \boldsymbol{\lambda}^T \mathbf{r}(\mathbf{u}; \mathbf{x})$$

First-order optimality (KKT) conditions for full space optimization problem

$$\nabla_{\mathbf{u}} \mathcal{L}(\mathbf{u}^*, \mathbf{x}^*, \boldsymbol{\lambda}^*) = \mathbf{0}, \quad \nabla_{\mathbf{x}} \mathcal{L}(\mathbf{u}^*, \mathbf{x}^*, \boldsymbol{\lambda}^*) = \mathbf{0}, \quad \nabla_{\boldsymbol{\lambda}} \mathcal{L}(\mathbf{u}^*, \mathbf{x}^*, \boldsymbol{\lambda}^*) = \mathbf{0}$$

Apply (quasi-)Newton method<sup>1</sup> to solve nonlinear KKT system for  $\mathbf{u}^*$ ,  $\mathbf{x}^*$ ,  $\boldsymbol{\lambda}^*$

---

<sup>1</sup>usually requires globalization such as linesearch or trust-region

# Implementation mostly requires standard terms in implicit code

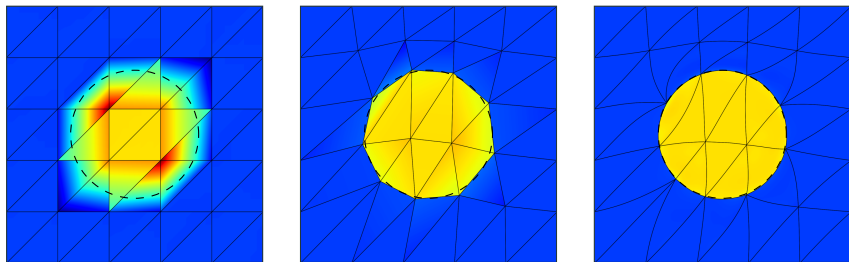
Gradient-based optimizers for the tracking optimization problem will require

$$\begin{array}{lll} f(\mathbf{u}, \mathbf{x}), & \frac{\partial f}{\partial \mathbf{u}}(\mathbf{u}, \mathbf{x}), & \frac{\partial f}{\partial \mathbf{x}}(\mathbf{u}, \mathbf{x}), \\ \mathbf{r}(\mathbf{u}, \mathbf{x}), & \frac{\partial \mathbf{r}}{\partial \mathbf{u}}(\mathbf{u}, \mathbf{x}), & \frac{\partial \mathbf{r}}{\partial \mathbf{x}}(\mathbf{u}, \mathbf{x}) \end{array}$$

- $\mathbf{r}$  and  $\partial_{\mathbf{u}}\mathbf{r}$  required by standard implicit solvers
- Same terms required for reduced space approach

# $L^2$ projection of discontinuous function on DG basis

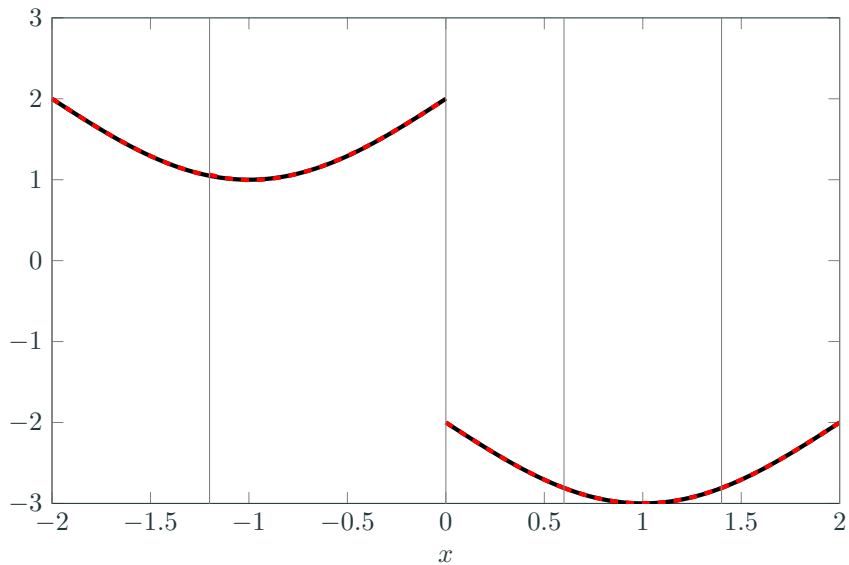
$$\eta(x) = \begin{cases} 2, & x^2 + y^2 < r^2 \\ 1, & x^2 + y^2 > r^2 \end{cases}$$



Non-aligned (*left*) vs. discontinuity-aligned mesh with linear (*middle*) and cubic (*right*) elements

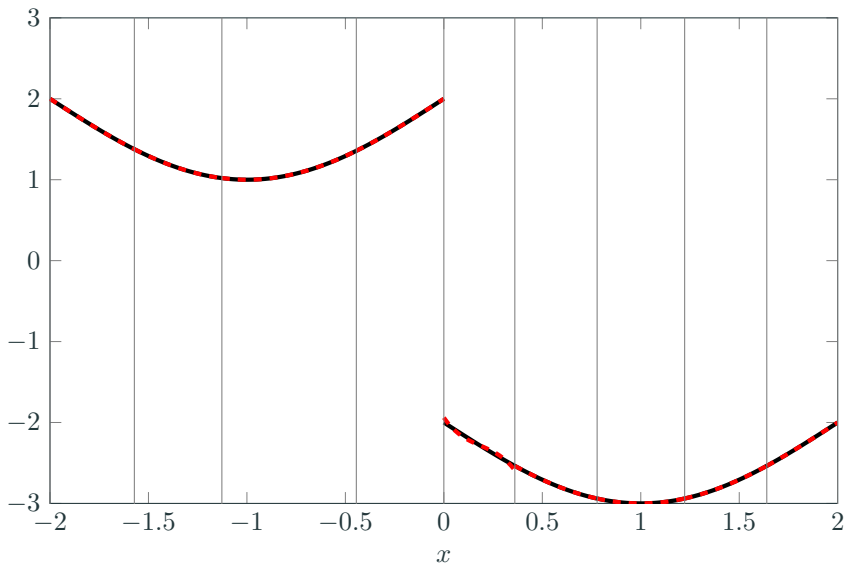


# Resolution of modified Burgers' equation with few elements



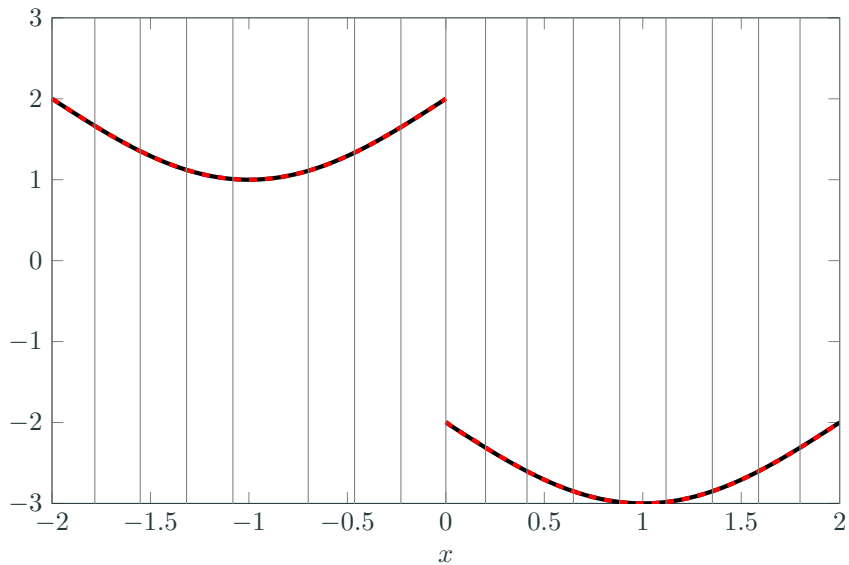
Exact solution (—), tracking solution (---) and mesh (—) for  $p = 3$

# Resolution of modified Burgers' equation with few elements



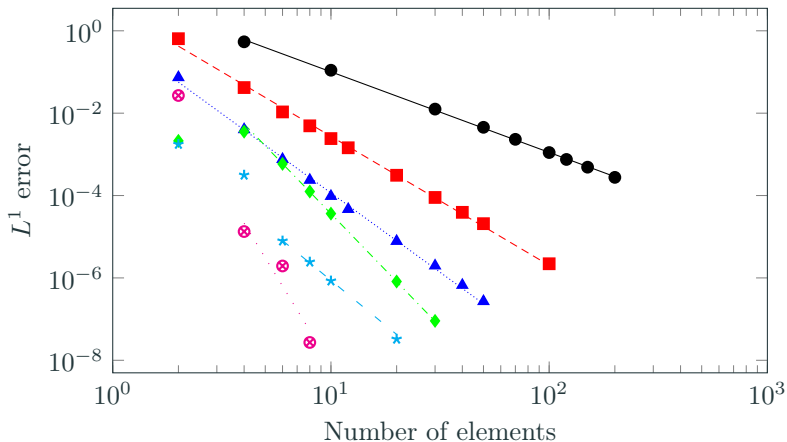
Exact solution (—), tracking solution (---) and mesh (—) for  $p = 3$

# Resolution of modified Burgers' equation with few elements



Exact solution (—), tracking solution (---) and mesh (|) for  $p = 3$

# $\mathcal{O}(h^{p+1})$ convergence rates demonstrated for Burgers' equation

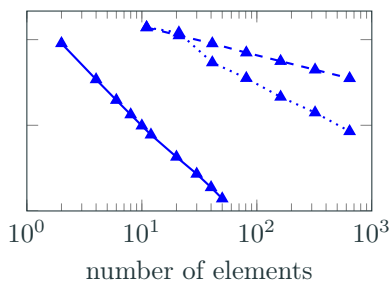
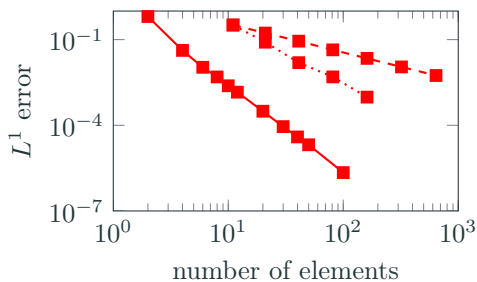
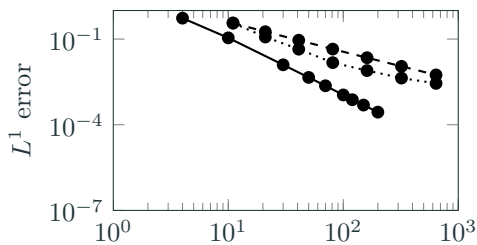


$p = 1$  (●),  $p = 2$  (■),  $p = 3$  (▲),  $p = 4$  (◆),  $p = 5$  (\*),  $p = 6$  (⊗)

The slopes of the best-fit lines to the data points in the asymptotic regime are:

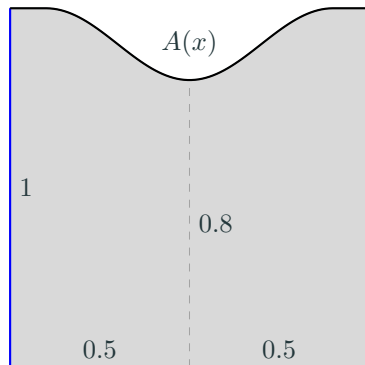
$\angle - 2.0$  (—),  $\angle - 3.1$  (- - -),  $\angle - 3.9$  (.....),  $\angle - 5.5$  (- · - ·),  $\angle - 4.4$  (- - -),  $\angle - 8.7$  (· · · ·)

# Convergence: tracking vs. uniform/adaptive refinement



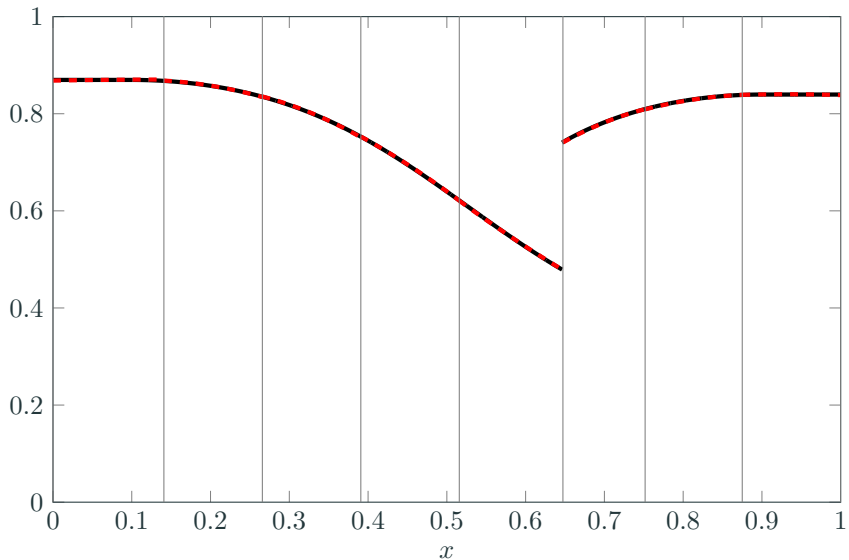
discontinuity-tracking	$p = 1$ (—●—)	$p = 2$ (—■—)	$p = 3$ (—▲—)
uniform refinement	$p = 1$ (-●-)	$p = 2$ (-■-)	$p = 3$ (-▲-)
adaptive refinement	$p = 1$ (··●··)	$p = 2$ (··■··)	$p = 3$ (··▲··)

# Nozzle flow: quasi-1d Euler equations



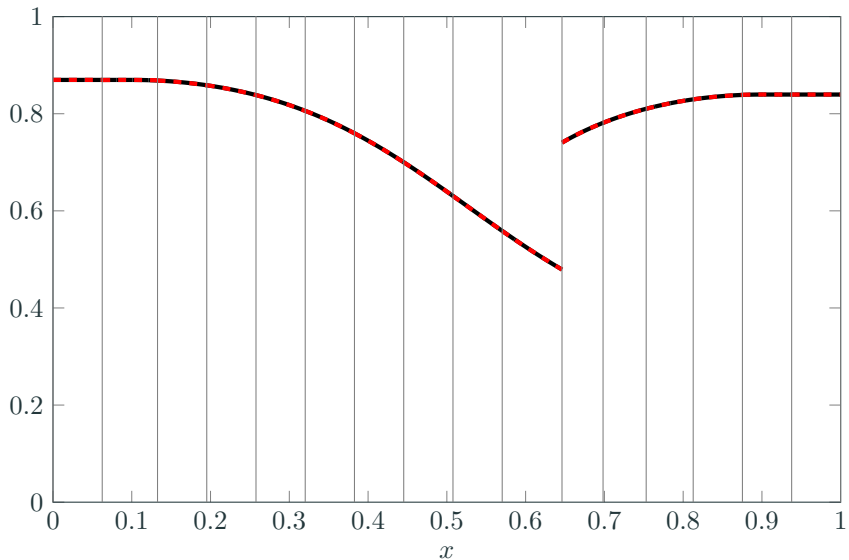
Inviscid wall (—), inflow (—), outflow (—)

# Resolution of quasi-1d Euler equations with few elements



Exact solution (—), tracking solution (---) and mesh (|) for  $p = 3$

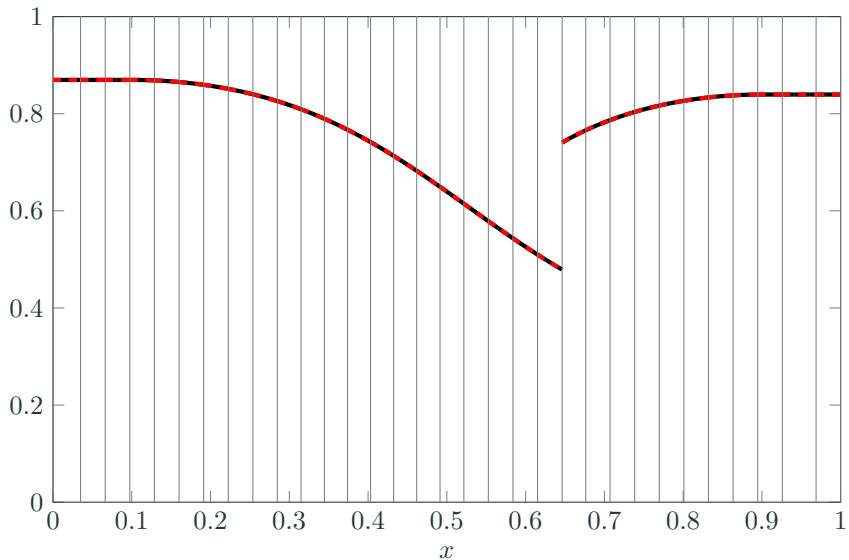
# Resolution of quasi-1d Euler equations with few elements



Exact solution (—), tracking solution (- - -) and mesh (|) for  $p = 3$

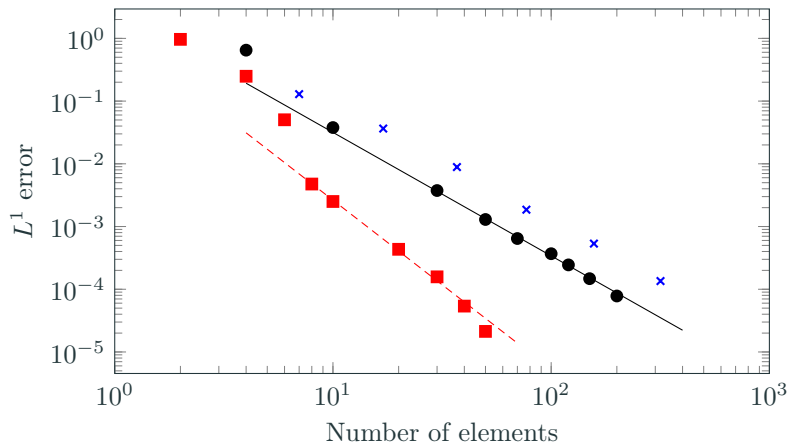


# Resolution of quasi-1d Euler equations with few elements



Exact solution (—), tracking solution (- - -) and mesh (—) for  $p = 3$

# $\mathcal{O}(h^{p+1})$ convergence rates demonstrated for nozzle flow

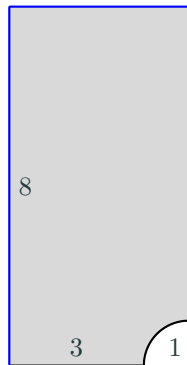


$p = 1$  (●),  $p = 2$  (■)

Slope of best-fit line:  $\angle -2.0$  (—),  $\angle -2.7$  (---)

Reference second-order method ( $p = 1$ ) with adaptive mesh refinement (×)

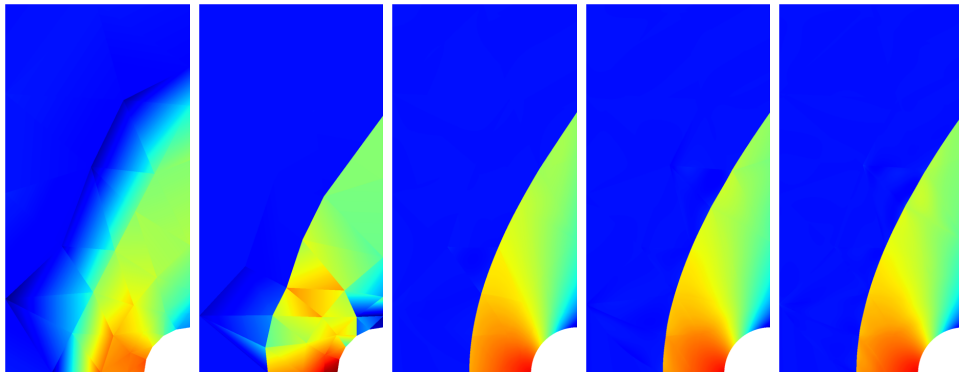
# Supersonic flow ( $M = 2$ ) around cylinder: 2D Euler equations



Inviscid wall/symmetry condition (—) and farfield (—)

# Resolution of 2D supersonic flow with 48 elements

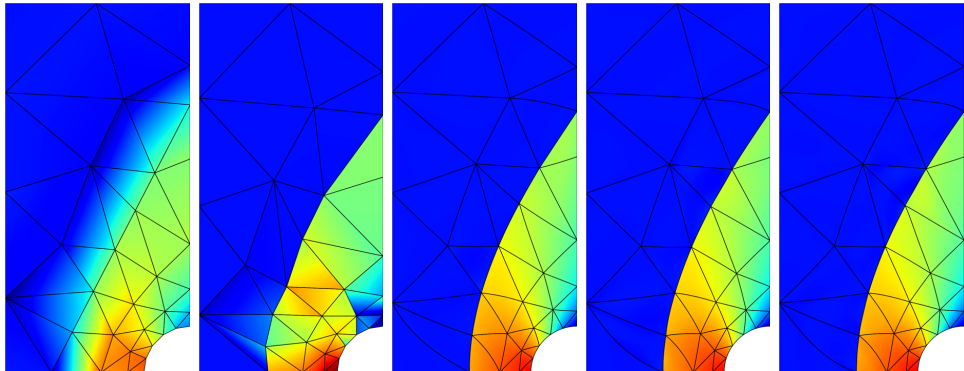
*Density ( $\rho$ )*



*Left:* Solution on non-aligned mesh with 48 linear elements and added viscosity (initial guess for shock tracking method). *Remaining:* solution using shock tracking framework corresponding to mesh with 48  $p = 1$ ,  $p = 2$ ,  $p = 3$ ,  $p = 4$  elements.

# Resolution of 2D supersonic flow with 48 elements

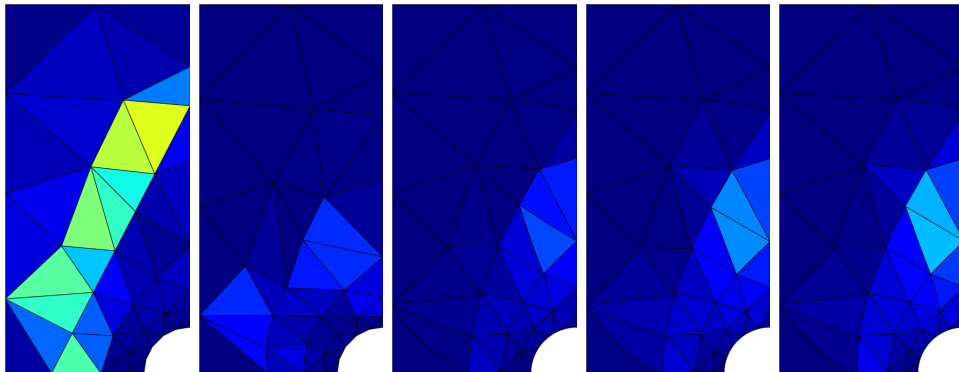
*Density ( $\rho$ )*



*Left:* Solution on non-aligned mesh with 48 linear elements and added viscosity (initial guess for shock tracking method). *Remaining:* solution using shock tracking framework corresponding to mesh with 48  $p = 1$ ,  $p = 2$ ,  $p = 3$ ,  $p = 4$  elements.

# Resolution of 2D supersonic flow with 48 elements

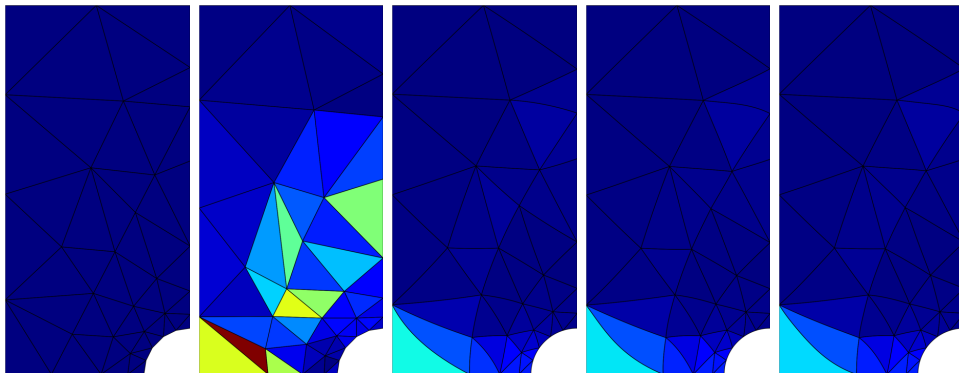
*Shock tracking objective ( $f_{shk}$ )*



*Left:* Solution on non-aligned mesh with 48 linear elements and added viscosity (initial guess for shock tracking method). *Remaining:* solution using shock tracking framework corresponding to mesh with 48  $p = 1$ ,  $p = 2$ ,  $p = 3$ ,  $p = 4$  elements.

# Resolution of 2D supersonic flow with 48 elements

*Distortion metric ( $f_{msh}$ )*



*Left:* Solution on non-aligned mesh with 48 linear elements and added viscosity (initial guess for shock tracking method). *Remaining:* solution using shock tracking framework corresponding to mesh with 48  $p = 1$ ,  $p = 2$ ,  $p = 3$ ,  $p = 4$  elements.

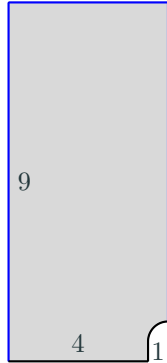
# Convergence to optimal solution and mesh



## Discontinuity-tracking performance summary

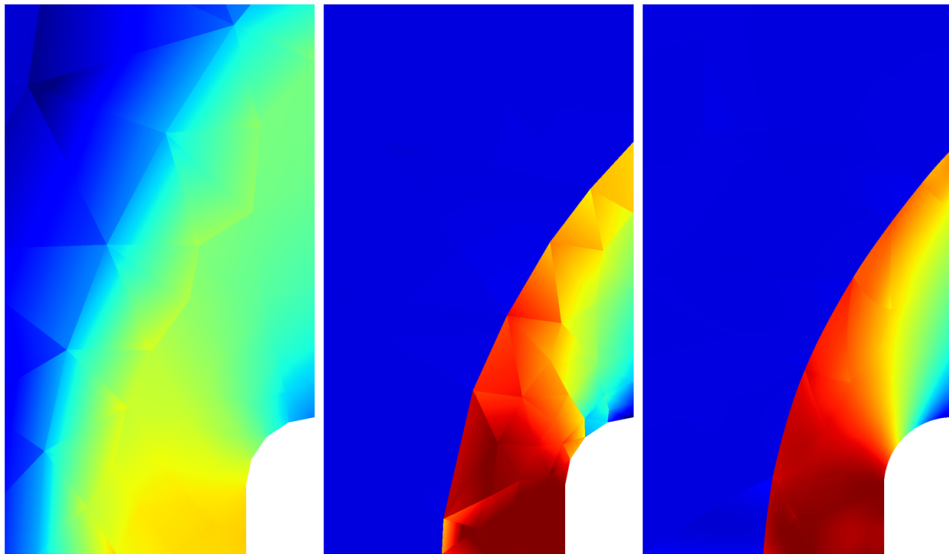
Polynomial order ( $p$ )	1	2	3	4
Degrees of freedom ( $N_{\mathbf{u}}$ )	576	1152	1920	2880
Enthalpy error ( $e_H$ )	0.0106	0.000462	0.00151	0.000885
Stagnation pressure error ( $e_p$ )	0.0711	0.00479	0.0112	0.000616

# Supersonic flow ( $M = 4$ ) around blunt body: 2D Euler equations



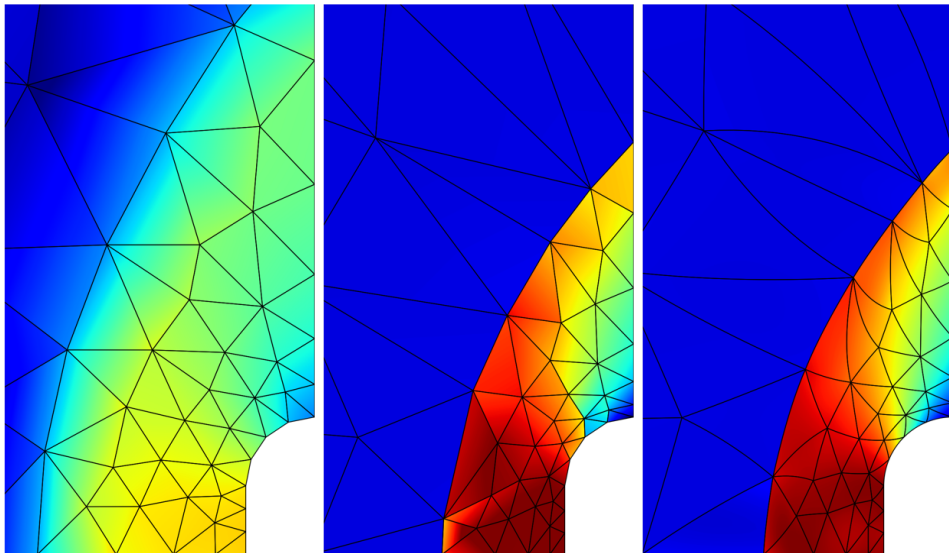
Inviscid wall/symmetry condition (—) and farfield (—)

## Resolution of 2D supersonic flow with 102 quadratic elements



*Left:* Solution (density) on non-aligned mesh with 102 linear elements and added viscosity (initial guess for shock tracking method). *Middle/right:* solution using shock tracking framework corresponding to mesh with 102 linear (*middle*) and quadratic (*right*) elements.

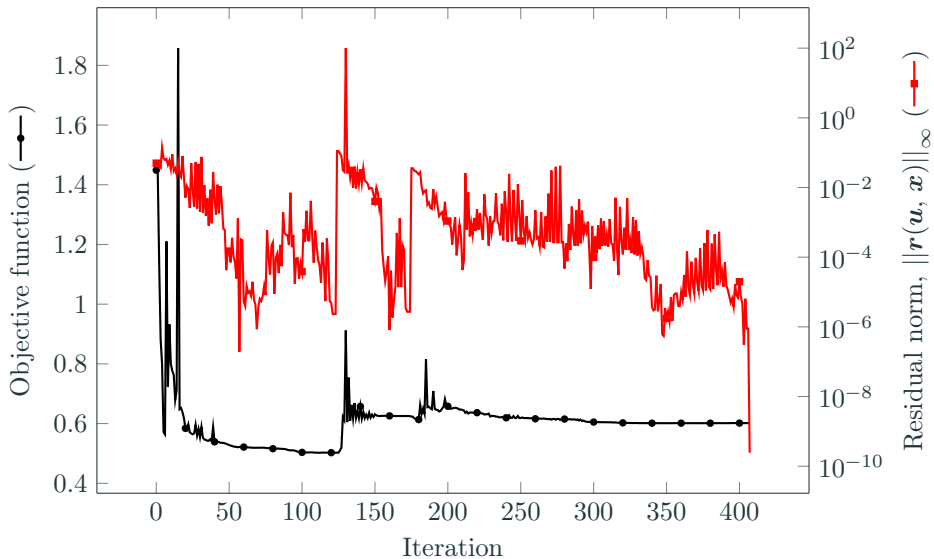
## Resolution of 2D supersonic flow with 102 quadratic elements



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# Convergence to optimal solution and mesh

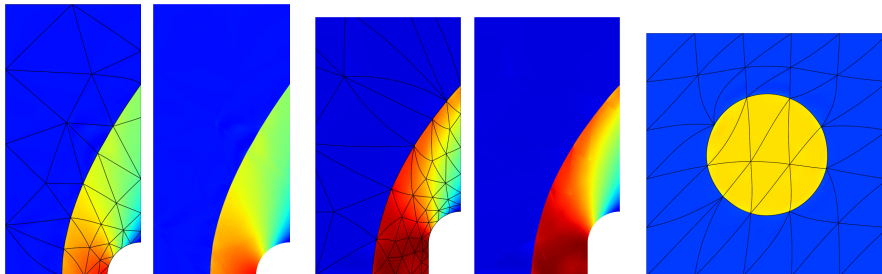
# Solver simultaneously minimizes objective and solves PDE






Convergence of residual and objective function

# Conclusions and future work

- Introduced high-order shock tracking method based on DG discretization and PDE-constrained optimization formulation
- Key innovations: *objective function* that monotonically approaches a minimum as mesh face aligns with shock and *full space solver*
- Optimal convergence  $\mathcal{O}(h^{p+1})$  rates obtained and used to resolve a number of transonic and supersonic flows on very coarse meshes
- Future work
  - **numerical flux** consistent with *integral form* (jumps do not tend to 0)
  - **solver** that exploits *problem structure* and incorporates *homotopy*
  - **local topology changes** to reduce iterations and improve mesh quality



Mach 2 flow around cylinder (*left*), Mach 4 flow around blunt body (*middle*), and  $L^2$  projection of discontinuous function (*right*).

-  Barter, G. E. (2008).  
*Shock capturing with PDE-based artificial viscosity for an adaptive, higher-order discontinuous Galerkin finite element method.*  
PhD thesis, M.I.T.
-  Huang, D. Z., Persson, P.-O., and Zahr, M. J. (2018).  
**High-order, linearly stable, partitioned solvers for general multiphysics problems based on implicit-explicit Runge-Kutta schemes.**  
*Computer Methods in Applied Mechanics and Engineering.*
-  Wang, J., Zahr, M. J., and Persson, P.-O. (6/5/2017 – 6/9/2017).  
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Zahr, M. J. and Persson, P.-O. (2016).

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*Journal of Computational Physics*, 326(Supplement C):516 – 543.



Zahr, M. J. and Persson, P.-O. (2018a).

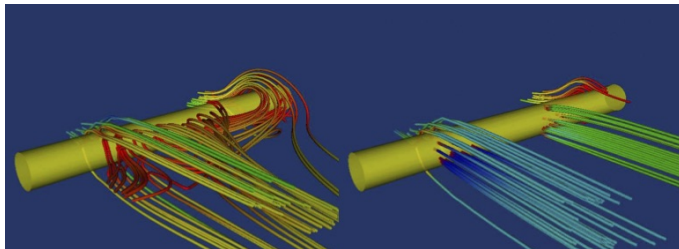
**An optimization-based approach for high-order accurate discretization of conservation laws with discontinuous solutions.**

*Journal of Computational Physics*, 365:105 – 134.

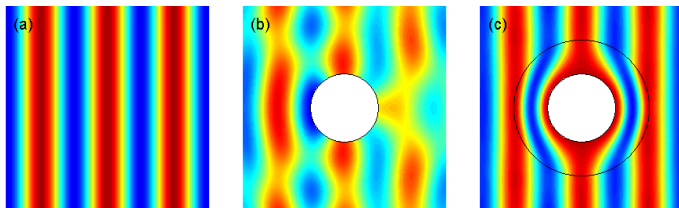
-  Zahr, M. J., Persson, P.-O., and Wilkening, J. (2016).  
**A fully discrete adjoint method for optimization of flow problems on deforming domains with time-periodicity constraints.**  
*Computers & Fluids*, 139:130 – 147.

# PDE optimization is ubiquitous in science and engineering

**Control:** Drive system to a desired state



Boundary flow control



Metamaterial cloaking – electromagnetic invisibility

# High-order discretization of PDE-constrained optimization

- *Continuous* PDE-constrained optimization problem

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

- *Fully discrete* PDE-constrained optimization problem

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

## Discrete adjoint equations can be derived from an algebraic manipulation to save computations

Let  $\mathbf{u}(\boldsymbol{\mu})$  be the solution of  $\mathbf{r}(\cdot, \boldsymbol{\mu}) = 0$

$$\mathbf{r}(\boldsymbol{\mu}) = \mathbf{r}(\mathbf{u}(\boldsymbol{\mu}), \boldsymbol{\mu}) = 0, \quad F(\boldsymbol{\mu}) = F(\mathbf{u}(\boldsymbol{\mu}), \boldsymbol{\mu})$$

## Discrete adjoint equations can be derived from an algebraic manipulation to save computations

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$$\mathbf{r}(\boldsymbol{\mu}) = \mathbf{r}(\mathbf{u}(\boldsymbol{\mu}), \boldsymbol{\mu}) = 0, \quad F(\boldsymbol{\mu}) = F(\mathbf{u}(\boldsymbol{\mu}), \boldsymbol{\mu})$$

The total derivative of  $\mathbf{r}$  leads to the sensitivity equations

$$D\mathbf{r} = \frac{\partial \mathbf{r}}{\partial \boldsymbol{\mu}} + \frac{\partial \mathbf{r}}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \boldsymbol{\mu}} = 0 \implies \frac{\partial \mathbf{u}}{\partial \boldsymbol{\mu}} = -\frac{\partial \mathbf{r}}{\partial \mathbf{u}}^{-1} \frac{\partial \mathbf{r}}{\partial \boldsymbol{\mu}}$$

# Discrete adjoint equations can be derived from an algebraic manipulation to save computations

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The total derivative of  $F$

$$DF = \frac{\partial F}{\partial \boldsymbol{\mu}} + \frac{\partial F}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \boldsymbol{\mu}}$$

# Discrete adjoint equations can be derived from an algebraic manipulation to save computations

Let  $\mathbf{u}(\boldsymbol{\mu})$  be the solution of  $\mathbf{r}(\cdot, \boldsymbol{\mu}) = 0$

$$\mathbf{r}(\boldsymbol{\mu}) = \mathbf{r}(\mathbf{u}(\boldsymbol{\mu}), \boldsymbol{\mu}) = 0, \quad F(\boldsymbol{\mu}) = F(\mathbf{u}(\boldsymbol{\mu}), \boldsymbol{\mu})$$

The total derivative of  $\mathbf{r}$  leads to the sensitivity equations

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The total derivative of  $F$

$$DF = \frac{\partial F}{\partial \boldsymbol{\mu}} + \frac{\partial F}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \boldsymbol{\mu}} = \frac{\partial F}{\partial \boldsymbol{\mu}} - \frac{\partial F}{\partial \mathbf{u}} \frac{\partial \mathbf{r}^{-1}}{\partial \mathbf{u}} \frac{\partial \mathbf{r}}{\partial \boldsymbol{\mu}}$$



## Discrete adjoint equations can be derived from an algebraic manipulation to save computations

Let  $\mathbf{u}(\boldsymbol{\mu})$  be the solution of  $\mathbf{r}(\cdot, \boldsymbol{\mu}) = 0$

$$\mathbf{r}(\boldsymbol{\mu}) = \mathbf{r}(\mathbf{u}(\boldsymbol{\mu}), \boldsymbol{\mu}) = 0, \quad F(\boldsymbol{\mu}) = F(\mathbf{u}(\boldsymbol{\mu}), \boldsymbol{\mu})$$

The total derivative of  $\mathbf{r}$  leads to the sensitivity equations

$$D\mathbf{r} = \frac{\partial \mathbf{r}}{\partial \boldsymbol{\mu}} + \frac{\partial \mathbf{r}}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \boldsymbol{\mu}} = 0 \implies \frac{\partial \mathbf{u}}{\partial \boldsymbol{\mu}} = -\frac{\partial \mathbf{r}^{-1}}{\partial \mathbf{u}} \frac{\partial \mathbf{r}}{\partial \boldsymbol{\mu}}$$

The total derivative of  $F$

$$DF = \frac{\partial F}{\partial \boldsymbol{\mu}} + \frac{\partial F}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \boldsymbol{\mu}} = \frac{\partial F}{\partial \boldsymbol{\mu}} - \frac{\partial F}{\partial \mathbf{u}} \frac{\partial \mathbf{r}^{-1}}{\partial \mathbf{u}} \frac{\partial \mathbf{r}}{\partial \boldsymbol{\mu}} = \frac{\partial F}{\partial \boldsymbol{\mu}} - \boldsymbol{\lambda}^T \frac{\partial \mathbf{r}}{\partial \boldsymbol{\mu}}$$

## Discrete adjoint equations can be derived from an algebraic manipulation to save computations

Let  $\mathbf{u}(\boldsymbol{\mu})$  be the solution of  $\mathbf{r}(\cdot, \boldsymbol{\mu}) = 0$

$$\mathbf{r}(\boldsymbol{\mu}) = \mathbf{r}(\mathbf{u}(\boldsymbol{\mu}), \boldsymbol{\mu}) = 0, \quad F(\boldsymbol{\mu}) = F(\mathbf{u}(\boldsymbol{\mu}), \boldsymbol{\mu})$$

The total derivative of  $\mathbf{r}$  leads to the sensitivity equations

$$D\mathbf{r} = \frac{\partial \mathbf{r}}{\partial \boldsymbol{\mu}} + \frac{\partial \mathbf{r}}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \boldsymbol{\mu}} = 0 \implies \frac{\partial \mathbf{u}}{\partial \boldsymbol{\mu}} = -\frac{\partial \mathbf{r}^{-1}}{\partial \mathbf{u}} \frac{\partial \mathbf{r}}{\partial \boldsymbol{\mu}}$$

The total derivative of  $F$

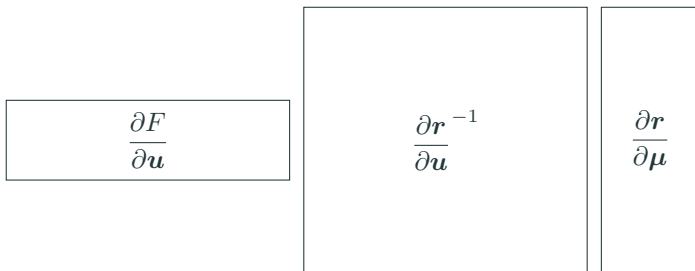
$$DF = \frac{\partial F}{\partial \boldsymbol{\mu}} + \frac{\partial F}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \boldsymbol{\mu}} = \frac{\partial F}{\partial \boldsymbol{\mu}} - \frac{\partial F}{\partial \mathbf{u}} \frac{\partial \mathbf{r}^{-1}}{\partial \mathbf{u}} \frac{\partial \mathbf{r}}{\partial \boldsymbol{\mu}} = \frac{\partial F}{\partial \boldsymbol{\mu}} - \boldsymbol{\lambda}^T \frac{\partial \mathbf{r}}{\partial \boldsymbol{\mu}}$$

Algebraic equations leads to adjoint equations

$$\frac{\partial \mathbf{r}^T}{\partial \mathbf{u}} \boldsymbol{\lambda} = \frac{\partial F^T}{\partial \mathbf{u}}$$

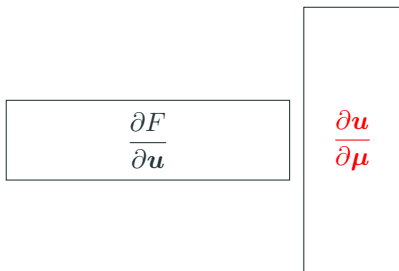
# Sensitivity vs. adjoint method to compute gradient of $F$

$$\frac{\partial F}{\partial \mathbf{u}} \frac{\partial \mathbf{r}^{-1}}{\partial \mathbf{u}} \frac{\partial \mathbf{r}}{\partial \boldsymbol{\mu}}$$



# Sensitivity vs. adjoint method to compute gradient of $F$

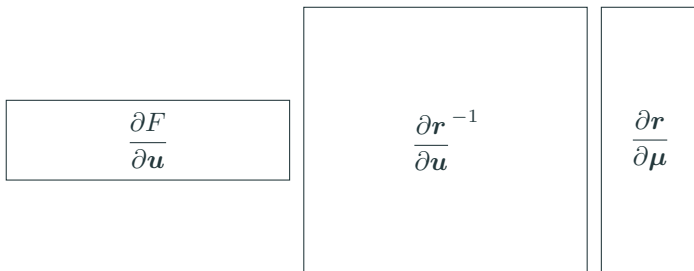
$$\frac{\partial F}{\partial \mathbf{u}} = \frac{\partial \mathbf{r}^{-1}}{\partial \mathbf{u}} \frac{\partial \mathbf{r}}{\partial \boldsymbol{\mu}}$$



Sensitivity method requires  $n_{\boldsymbol{\mu}}$  linear solves and  $n_F n_{\boldsymbol{\mu}}$  inner products ( $\mathbb{R}^{n_u}$ )

# Sensitivity vs. adjoint method to compute gradient of $F$

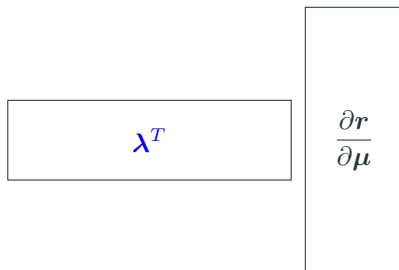
$$\frac{\partial F}{\partial \mathbf{u}} \frac{\partial \mathbf{r}^{-1}}{\partial \mathbf{u}} \frac{\partial \mathbf{r}}{\partial \boldsymbol{\mu}}$$



Sensitivity method requires  $n_{\boldsymbol{\mu}}$  linear solves and  $n_F n_{\boldsymbol{\mu}}$  inner products ( $\mathbb{R}^{n_u}$ )

# Sensitivity vs. adjoint method to compute gradient of $F$

$$\frac{\partial F}{\partial \mathbf{u}} \frac{\partial \mathbf{r}^{-1}}{\partial \mathbf{u}} \frac{\partial \mathbf{r}}{\partial \boldsymbol{\mu}}$$



Sensitivity method requires  $n_{\boldsymbol{\mu}}$  linear solves and  $n_F n_{\boldsymbol{\mu}}$  inner products ( $\mathbb{R}^{n_u}$ )

Adjoint method requires  $n_F$  linear solves and  $n_F n_{\boldsymbol{\mu}}$  inner products ( $\mathbb{R}^{n_u}$ )

# Adjoint equation derivation: outline

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

$$\begin{array}{l} \text{minimize} \\ \mathbf{u}_0, \dots, \mathbf{u}_{N_t} \in \mathbb{R}^{N_u}, \\ \mathbf{k}_{1,1}, \dots, \mathbf{k}_{N_t,s} \in \mathbb{R}^{N_u} \end{array} \quad F(\mathbf{u}_0, \dots, \mathbf{u}_{N_t}, \mathbf{k}_{1,1}, \dots, \mathbf{k}_{N_t,s}, \boldsymbol{\mu})$$

$$\text{subject to} \quad \mathbf{R}_0 = \mathbf{u}_0 - \mathbf{g}(\boldsymbol{\mu}) = 0$$

$$\mathbf{R}_n = \mathbf{u}_n - \mathbf{u}_{n-1} - \sum_{i=1}^s b_i \mathbf{k}_{n,i} = 0$$

$$\mathbf{R}_{n,i} = M \mathbf{k}_{n,i} - \Delta t_n \mathbf{r}(\mathbf{u}_{n,i}, \boldsymbol{\mu}, t_{n,i}) = 0$$

- Define **Lagrangian**

$$\mathcal{L}(\mathbf{u}_n, \mathbf{k}_{n,i}, \boldsymbol{\lambda}_n, \boldsymbol{\kappa}_{n,i}) = F - \boldsymbol{\lambda}_0^T \mathbf{R}_0 - \sum_{n=1}^{N_t} \boldsymbol{\lambda}_n^T \mathbf{R}_n - \sum_{n=1}^{N_t} \sum_{i=1}^s \boldsymbol{\kappa}_{n,i}^T \mathbf{R}_{n,i}$$

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

$$\frac{\partial \mathcal{L}}{\partial \mathbf{u}_n} = 0, \quad \frac{\partial \mathcal{L}}{\partial \mathbf{k}_{n,i}} = 0, \quad \frac{\partial \mathcal{L}}{\partial \boldsymbol{\lambda}_n} = 0, \quad \frac{\partial \mathcal{L}}{\partial \boldsymbol{\kappa}_{n,i}} = 0$$

High-quality reconstruction from coarse MRI grid (space:  $24 \times 36$ , time: 20) and low noise (3%)

Reconstructed flow

Synthetic MRI data  $\mathbf{d}_{i,n}^*$  (top) and  
computational representation of MRI  
data  $\mathbf{d}_{i,n}$  (bottom)



# High-quality reconstruction from fine MRI grid (space: $40 \times 60$ , time: 20) and low noise (3%)

Reconstructed flow

Synthetic MRI data  $\mathbf{d}_{i,n}^*$  (top) and  
computational representation of MRI  
data  $\mathbf{d}_{i,n}$  (bottom)

# Extension: constraint requiring time-periodicity [Zahr et al., 2016]

Optimization of *cyclic* problems requires finding time-periodic solution of PDE; necessary for physical relevance and avoid transients that may lead to crash

$$\text{minimize}_{\mathbf{U}, \boldsymbol{\mu}} \mathcal{F}(\mathbf{U}, \boldsymbol{\mu})$$

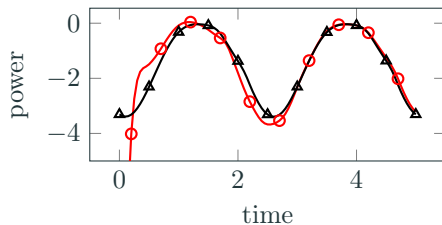
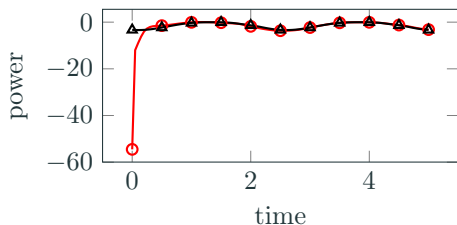
$$\text{subject to } \mathbf{U}(\mathbf{x}, 0) = \mathbf{U}(\mathbf{x}, T)$$

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{U}, \nabla \mathbf{U}) = 0$$

$$\boldsymbol{\lambda}_{N_t} = \boldsymbol{\lambda}_0 + \frac{\partial \mathcal{F}}{\partial \mathbf{u}_{N_t}}^T$$

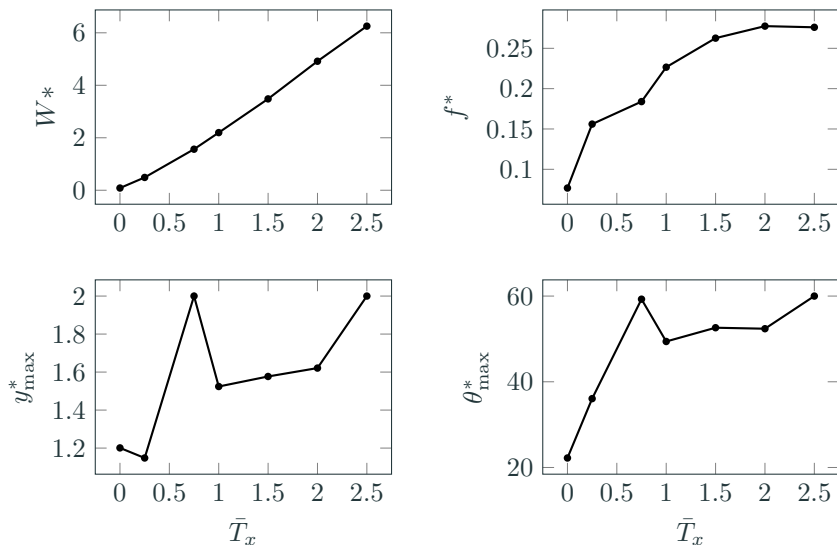
$$\boldsymbol{\lambda}_{n-1} = \boldsymbol{\lambda}_n + \frac{\partial \mathcal{F}}{\partial \mathbf{u}_{n-1}}^T + \sum_{i=1}^s \Delta t_n \frac{\partial \mathbf{r}_{n,i}}{\partial \mathbf{u}}^T \boldsymbol{\kappa}_{n,i}$$

$$\mathbf{M}^T \boldsymbol{\kappa}_{n,i} = \frac{\partial \mathcal{F}}{\partial \mathbf{u}_{N_t}}^T + b_i \boldsymbol{\lambda}_n + \sum_{j=i}^s a_{ji} \Delta t_n \frac{\partial \mathbf{r}_{n,i}}{\partial \mathbf{u}}^T \boldsymbol{\kappa}_{n,j}$$



Time history of power on airfoil of flow initialized from steady-state ( $\circ$ ) and from a time-periodic solution ( $\blacktriangle$ )

# Energetically optimal flapping vs. required thrust: QoI



The optimal flapping energy ( $W^*$ ), frequency ( $f^*$ ), maximum heaving amplitude ( $y_{\max}^*$ ), and maximum pitching amplitude ( $\theta_{\max}^*$ ) as a function of the thrust constraint  $\bar{T}_x$ .

## Initial guess for optimization: $\mathbf{u}_0, \phi_0$

- Initial guess for  $\mathbf{u}$  and  $\phi$  critical given the non-convex nonlinear optimization formulation of our shock tracking method
- *Homotopy*: define a sequence of shock tracking problems where the solution of problem  $j$  is used to initialize problem  $j + 1$
- Sequence of problems chosen using homotopy in *polynomial order* and Mach number (for high Mach flows)
- For initial problem in homotopy sequence:
  - $\phi_0$  chosen such that resulting mesh is identical to the reference mesh
  - $\mathbf{u}_0$  chosen as the solution of the discrete conservation law with enough added viscosity  $\nu$

$$\mathbf{r}_\nu(\mathbf{u}, \mathbf{x}(\phi_0)) = 0$$

# Modified Burgers' equation with discontinuous source term

Inviscid, modified one-dimensional Burgers' equation with a discontinuous source term from [Barter, 2008]

$$\frac{\partial}{\partial x} \left( \frac{1}{2} u^2 \right) = \beta u + f(x), \quad \text{for } x \in \Omega = (-2, 2),$$

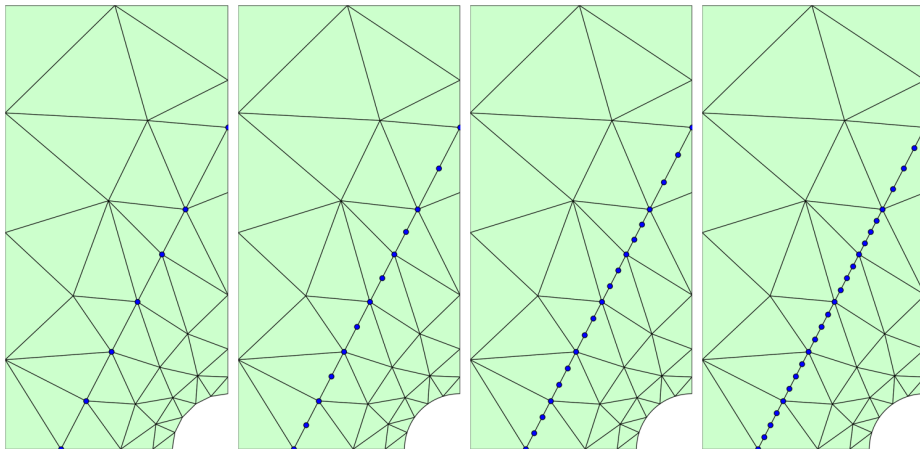
where  $u(-2) = 2$ ,  $u(2) = -2$ ,  $\beta = -0.1$  and

$$f(x) = \begin{cases} (2 + \sin(\frac{\pi x}{2}))(\frac{\pi}{2} \cos(\frac{\pi x}{2}) - \beta), & x < 0 \\ (2 + \sin(\frac{\pi x}{2}))(\frac{\pi}{2} \cos(\frac{\pi x}{2}) + \beta), & x > 0 \end{cases}$$

Analytical solution

$$u(x) = \begin{cases} 2 + \sin(\frac{\pi x}{2}), & x < 0 \\ -2 - \sin(\frac{\pi x}{2}), & x > 0 \end{cases}$$

# High-order meshes and parametrization



Reference domain and mesh with 48 elements and polynomial orders  $p = 1$  (*left*),  $p = 2$  (*middle left*),  $p = 3$  (*middle right*), and  $p = 4$  (*right*). The blue circles identify parametrized nodes.