

Integrated computational physics and numerical optimization

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September 21, 2018

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Integrating computational physics and numerical optimization

Optimize physics

Optimize numerics

Integrating computational physics and numerical optimization

Optimize physics

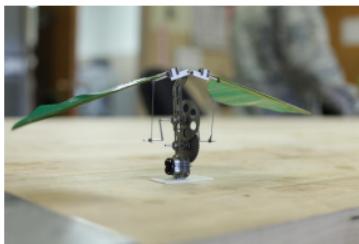
Optimize numerics

PDE optimization is ubiquitous in science and engineering

Design: Find system that optimizes performance metric, satisfies constraints



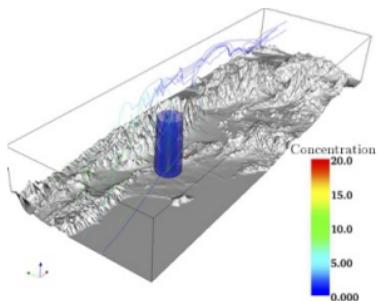
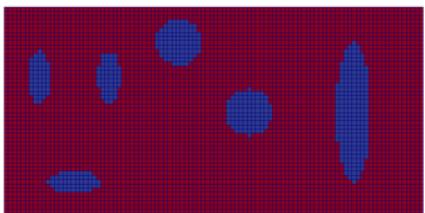
Aerodynamic shape design of automobile



Optimal flapping motion of micro aerial vehicle

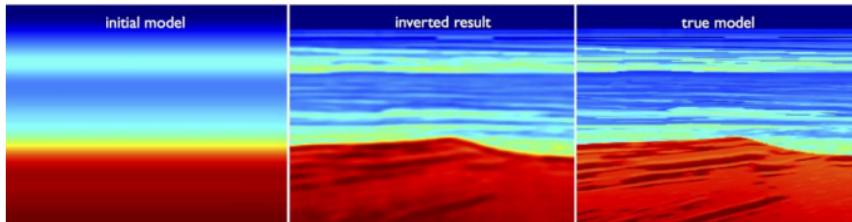
PDE optimization is ubiquitous in science and engineering

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

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

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

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

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

$$\boldsymbol{\mu}$$

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

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

PDE solution

design/control parameters

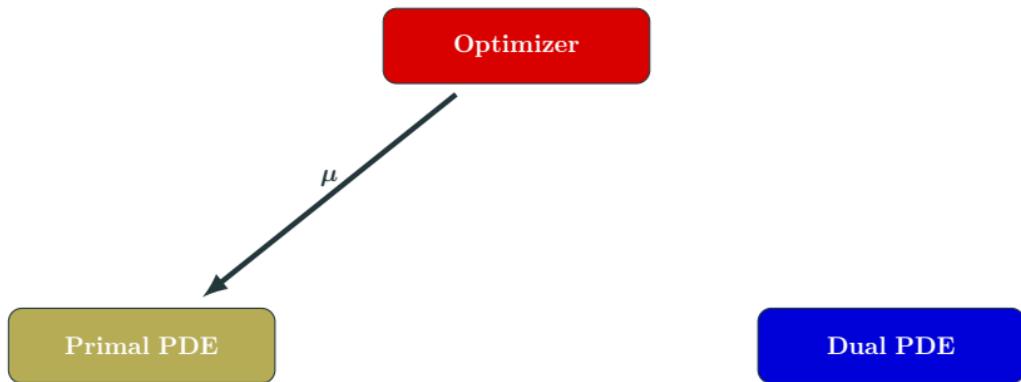
objective function

constraints

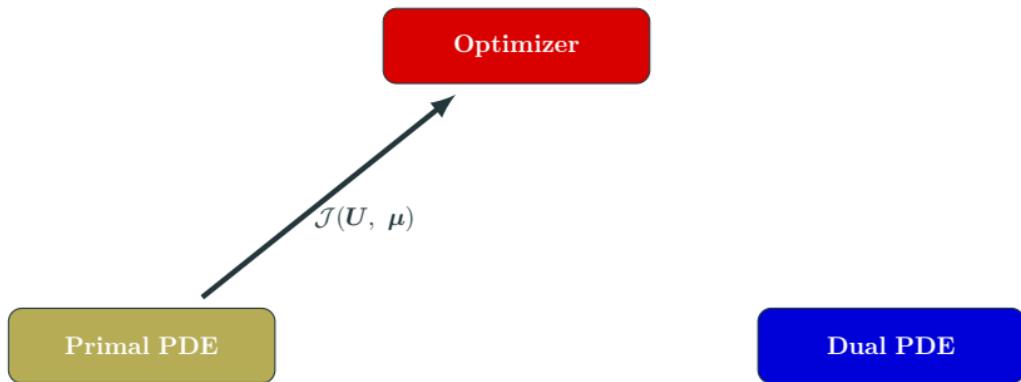
Nested approach to PDE-constrained optimization



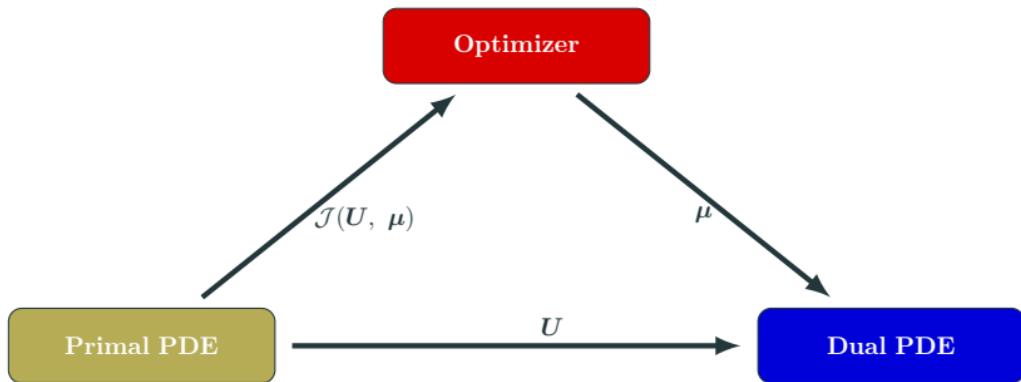
Nested approach to PDE-constrained optimization



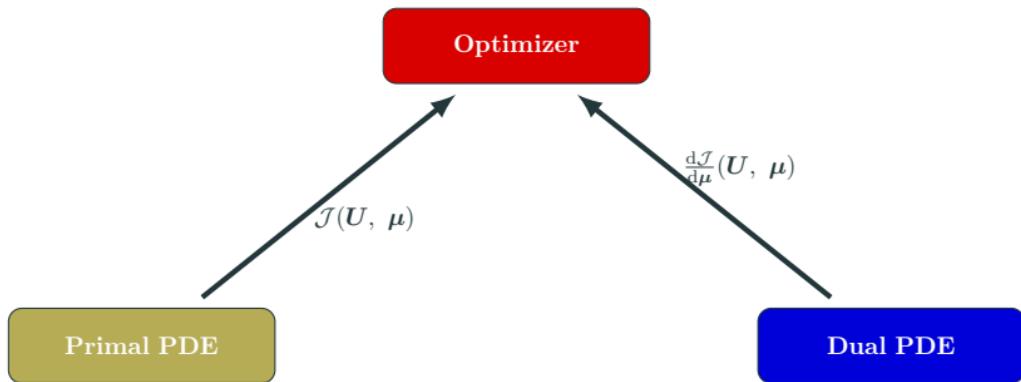
Nested approach to PDE-constrained optimization



Nested approach to PDE-constrained optimization



Nested approach to PDE-constrained optimization



Highlights of globally high-order discretization

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

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

Space discretization: discontinuous Galerkin

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

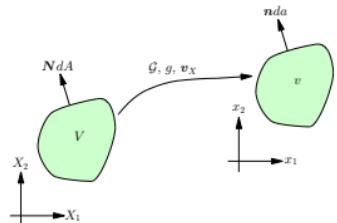
Time discretization: diagonally implicit RK

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

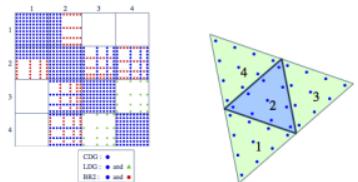
$$M \mathbf{k}_{n,i} = \Delta t_n \mathbf{r}(\mathbf{u}_{n,i}, \mu, t_{n,i})$$

Quantity of interest: solver-consistency

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



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**

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

Adjoint method to efficiently compute gradients of QoI

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

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

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 ouput**

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

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

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

Gradient reconstruction via dual variables

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

[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
 $T_x = 2.5$

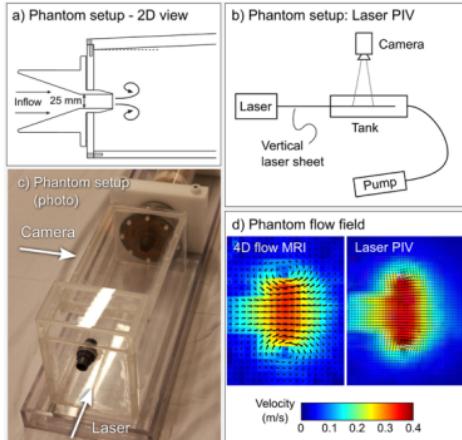
Optimal RBM/TMG
 $T_x = 2.5$

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

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

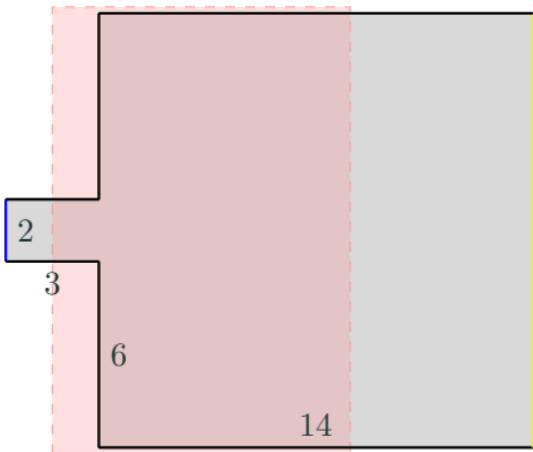
$$\chi_t(s; c, w) = \frac{1}{1 + e^{-(s-(c-0.5w))/\sigma}} - \frac{1}{1 + e^{-(s-(c+0.5w))/\sigma}}$$

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

\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, Δt 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: 24×36 , time: 10) and low noise (3%)

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

Reconstructed flow

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

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

Reconstructed flow

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

$$M_0 \dot{u}_0 = r_0(u_0, c_0(u_0, u_1))$$

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However, to solve in partitioned manner and achieve high-order, split as follows
and apply **implicit-explicit** Runge-Kutta

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Adjoint equations inherit **explicit-implicit** structure

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

Particle-laden flow

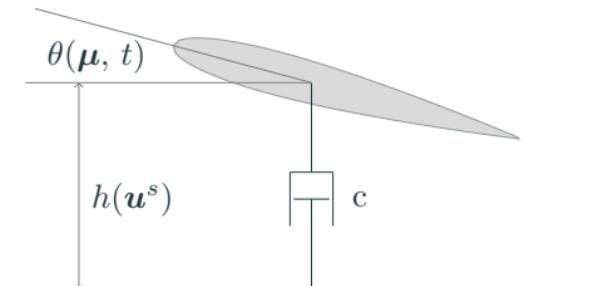
Fluid-structure interaction

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

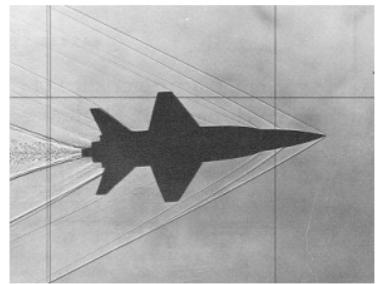
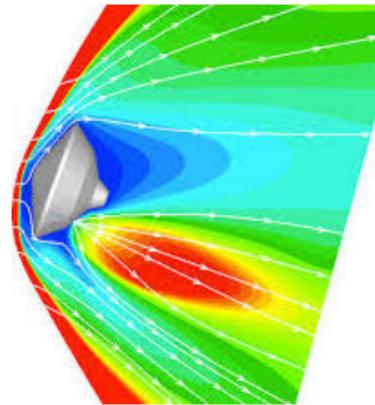
Optimize physics

Optimize numerics

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

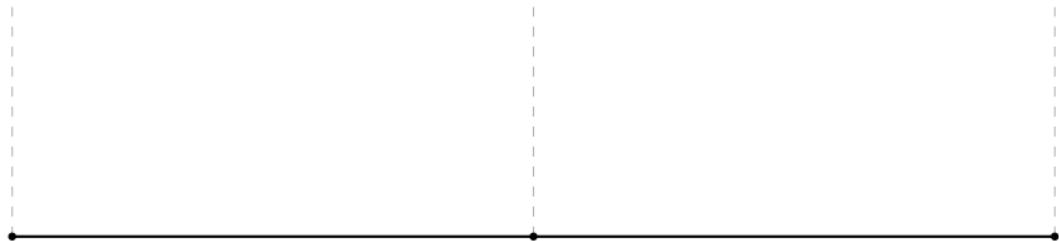
Supersonic and transonic flow around commercial planes and fighter jets

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



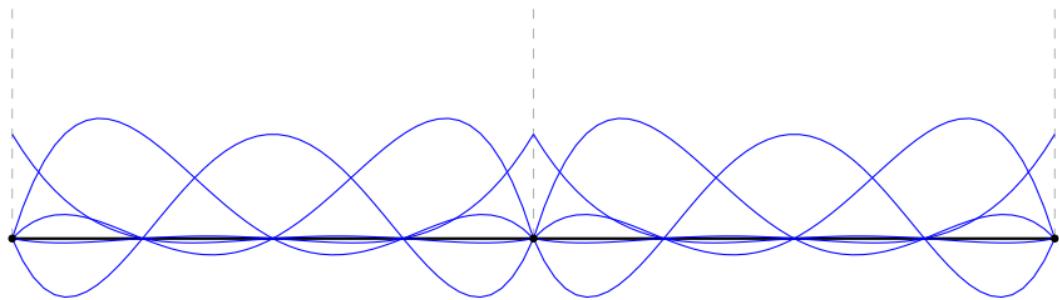
Other applications with discontinuities: fracture, problems with interfaces

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



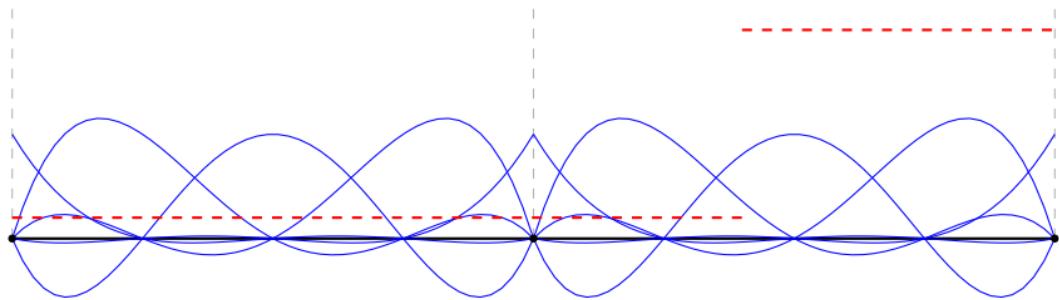
Fundamental issue: approximate discontinuity with polynomial basis

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



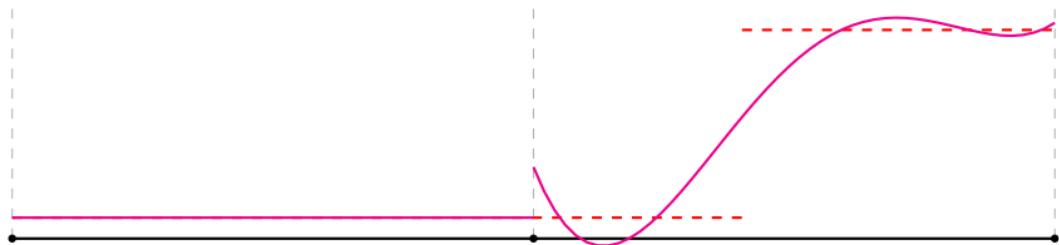
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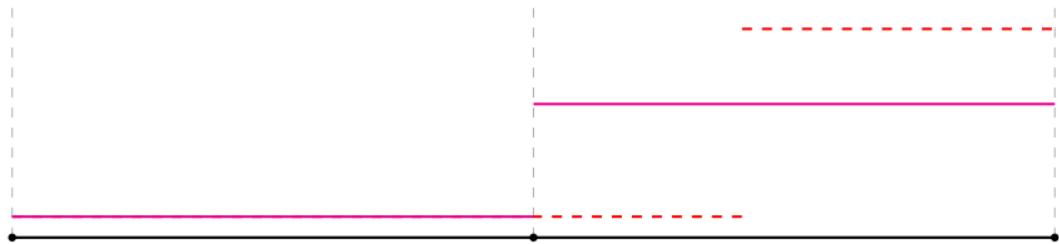
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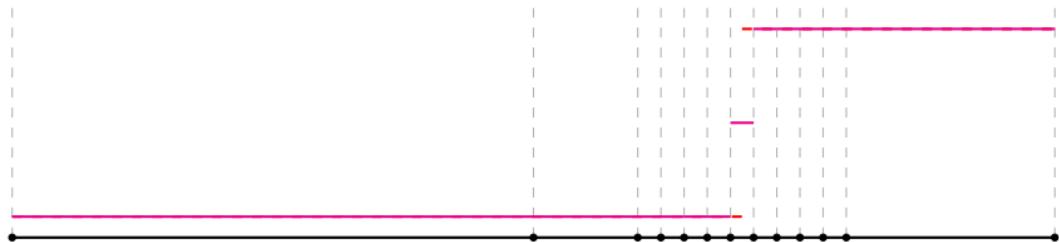


Fundamental issue: approximate discontinuity with polynomial basis

Existing solutions: **limiting**, artificial viscosity

Drawbacks: order reduction, local refinement

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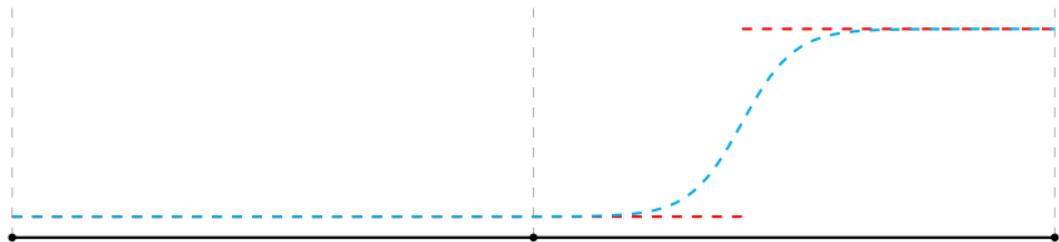


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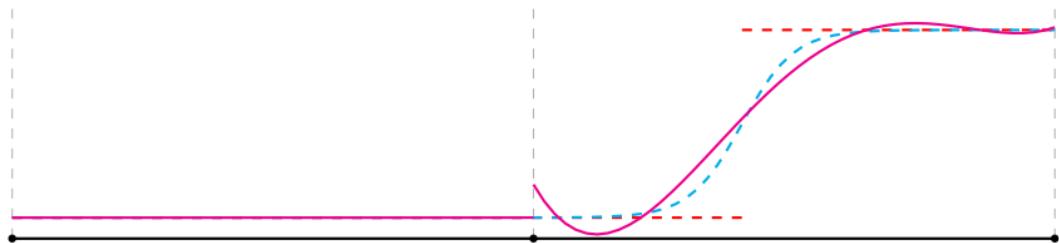


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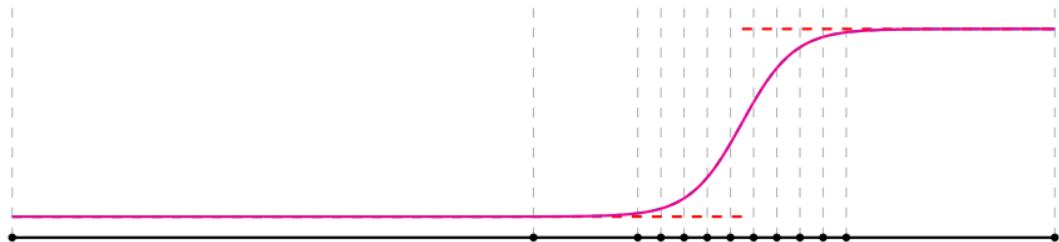


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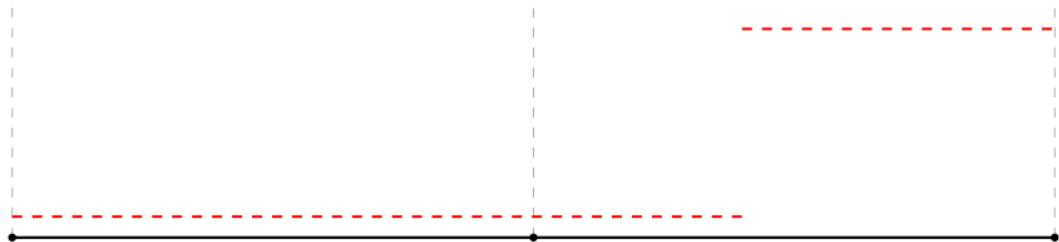


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Proposed solution: align features of solution basis with features in the solution using optimization formulation and solver

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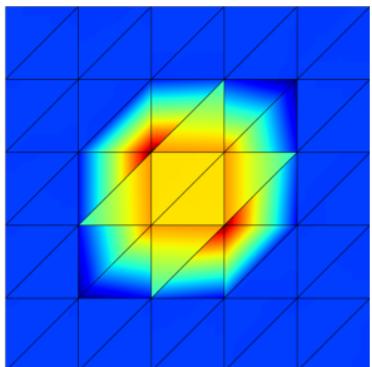
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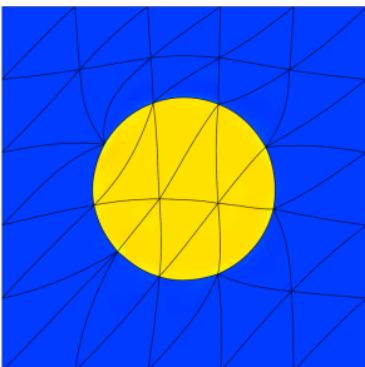
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Tracking method for stable, high-order resolution of discontinuities

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



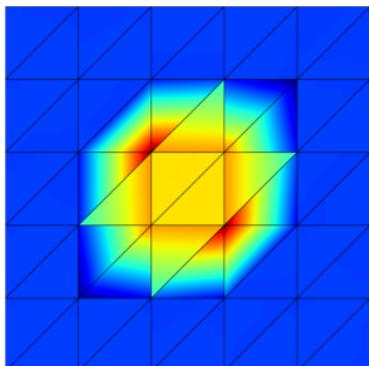
Non-aligned



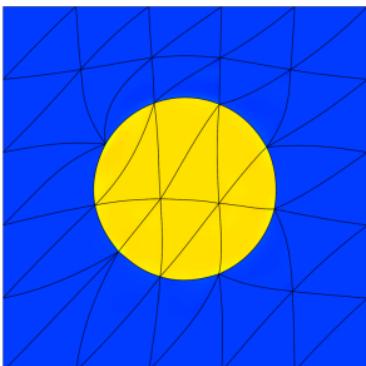
Discontinuity-aligned

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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

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

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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

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

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

Transformed conservation law from deformation of physical domain

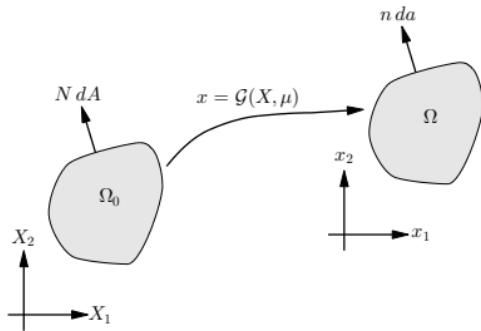
Consider physical domain as the result of a μ -parametrized diffeomorphism applied to some reference domain Ω_0

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

Re-write conservation law on reference domain

$$\nabla \cdot \mathcal{F}(U) = 0 \quad \text{in } \mathcal{G}(\Omega_0, \mu) \implies \nabla_X \cdot F(u, \mu) = 0 \quad \text{in } \Omega_0,$$

$$u = g_\mu U, \quad F(u, \mu) = g_\mu \mathcal{F}(g_\mu^{-1} u) G_\mu^{-T}, \quad G_\mu = \frac{\partial}{\partial X} \mathcal{G}(X, \mu), \quad g_\mu = \det G_\mu$$



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

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

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

Objective function: penalize oscillations and mesh distortion

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

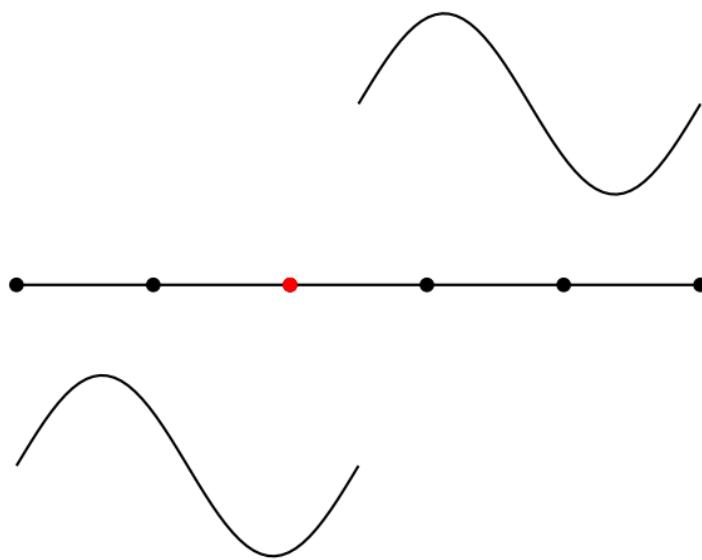
$$f_{shk}(\mathbf{u}, \mathbf{x}) = h_0^{-2} \sum_{K \in \mathcal{E}_{h,p}} \int_{\mathcal{G}(K, \mathbf{x})} \left\| u_{h,p} - \bar{u}_{h,p}^K \right\|_{\mathbf{W}}^2 dV,$$

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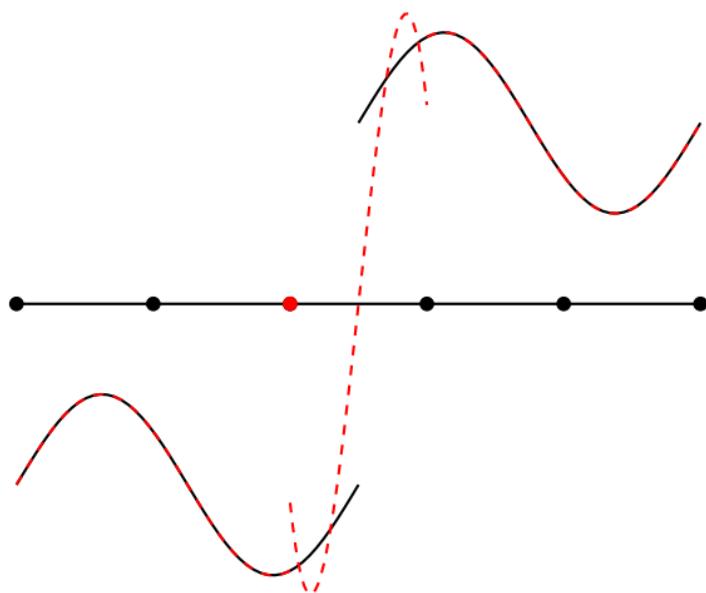
Construct objective function as weighted combination between discontinuity indicator and mesh distortion metric

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

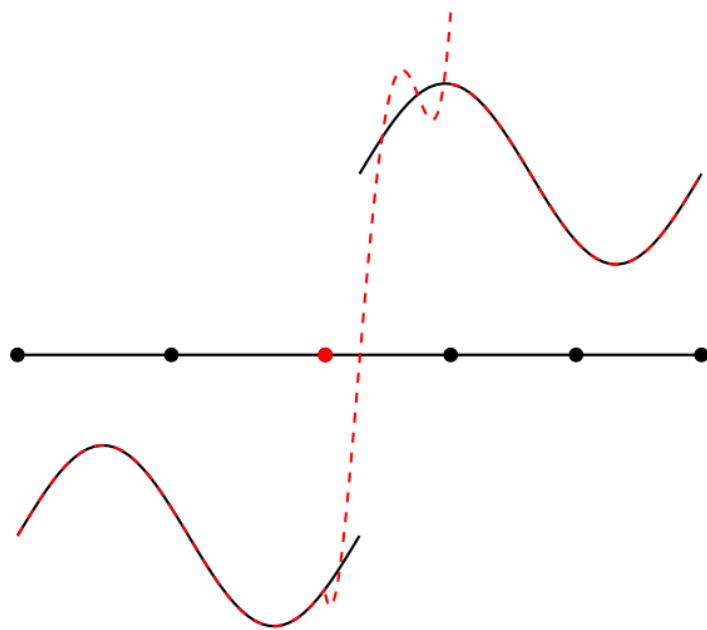
One-dimensional mesh parametrization and objective function test



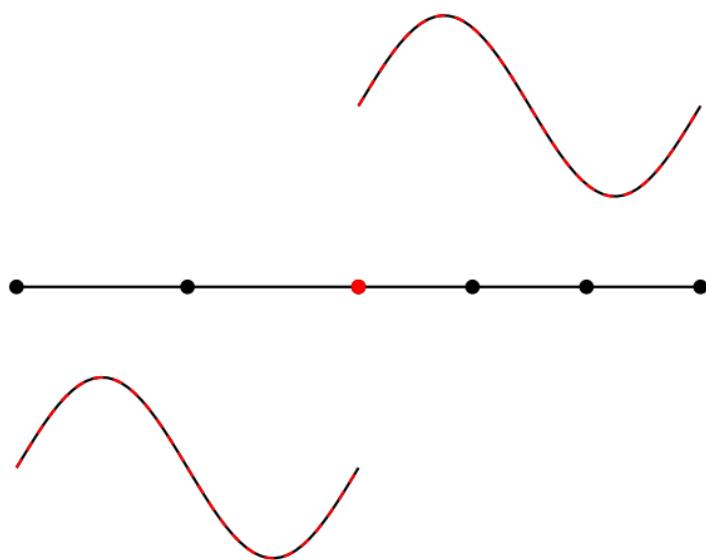
One-dimensional mesh parametrization and objective function test



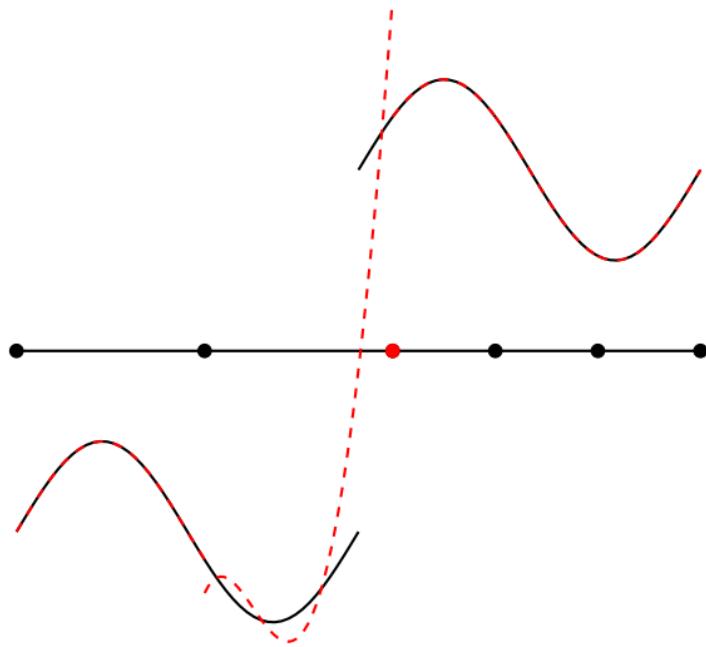
One-dimensional mesh parametrization and objective function test



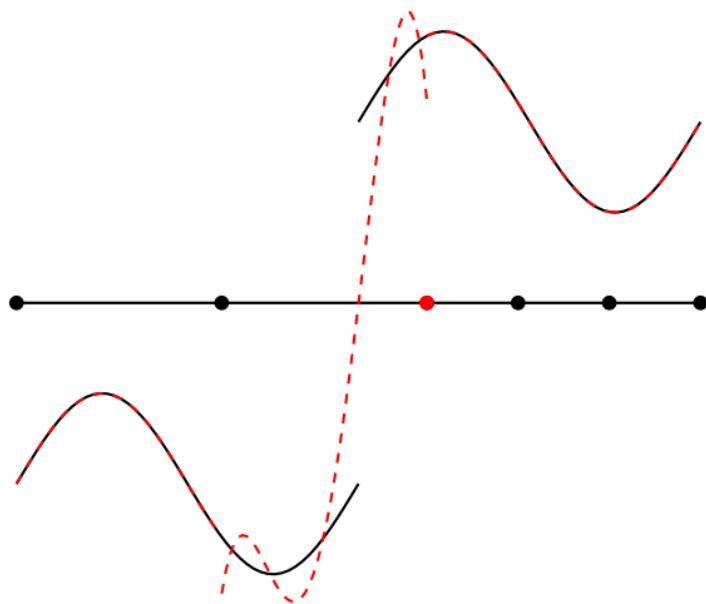
One-dimensional mesh parametrization and objective function test



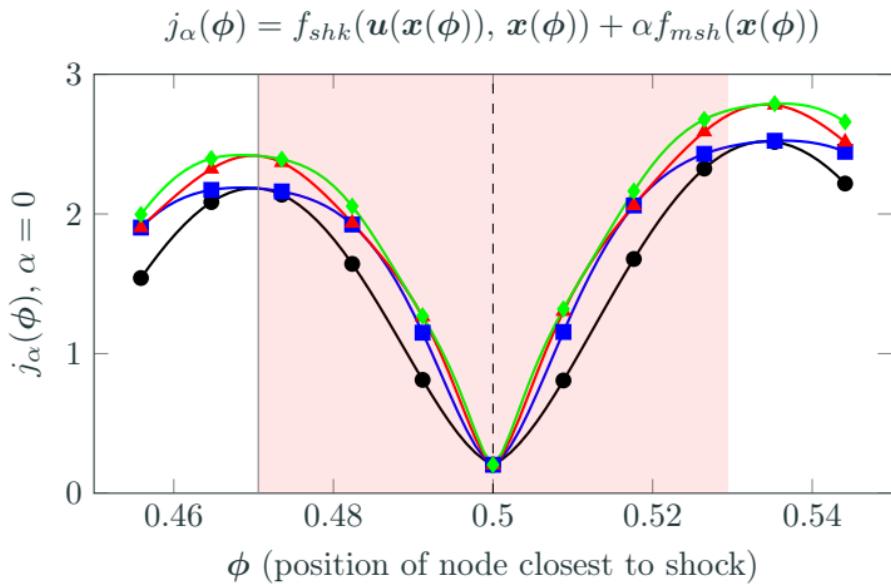
One-dimensional mesh parametrization and objective function test



One-dimensional mesh parametrization and objective function test

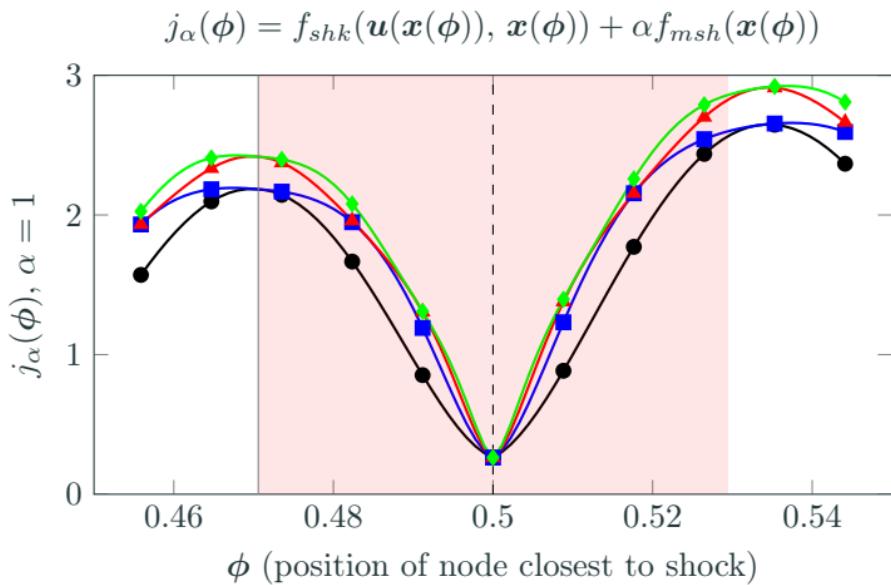


Objective function monotonically approaches minimum as mesh aligns with discontinuity, regardless of p , for a range of α



Objective function as an element face is smoothly swept across discontinuity (---):
 $p = 1$ (—●—), $p = 2$ (—■—), $p = 3$ (—▲—), $p = 4$ (—◆—).

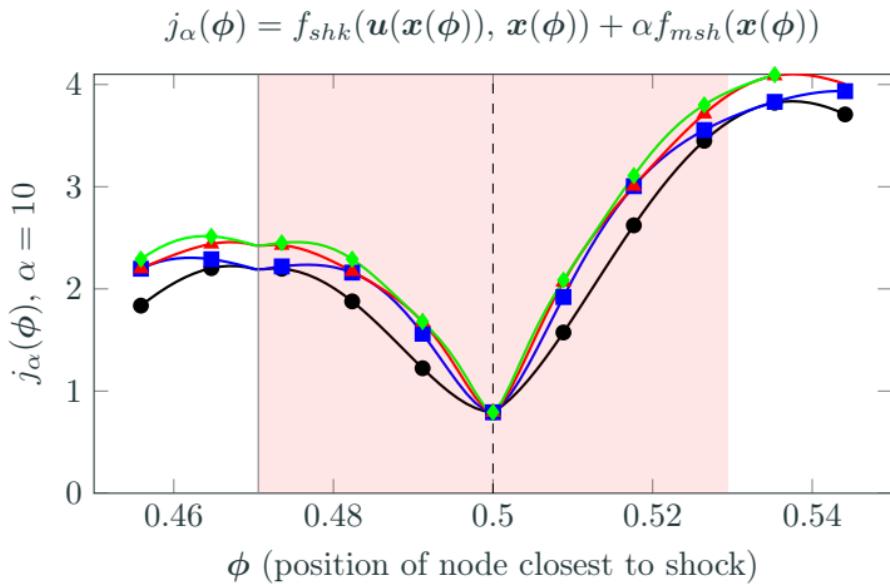
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$p = 1$ (●), $p = 2$ (■), $p = 3$ (▲), $p = 4$ (◆).

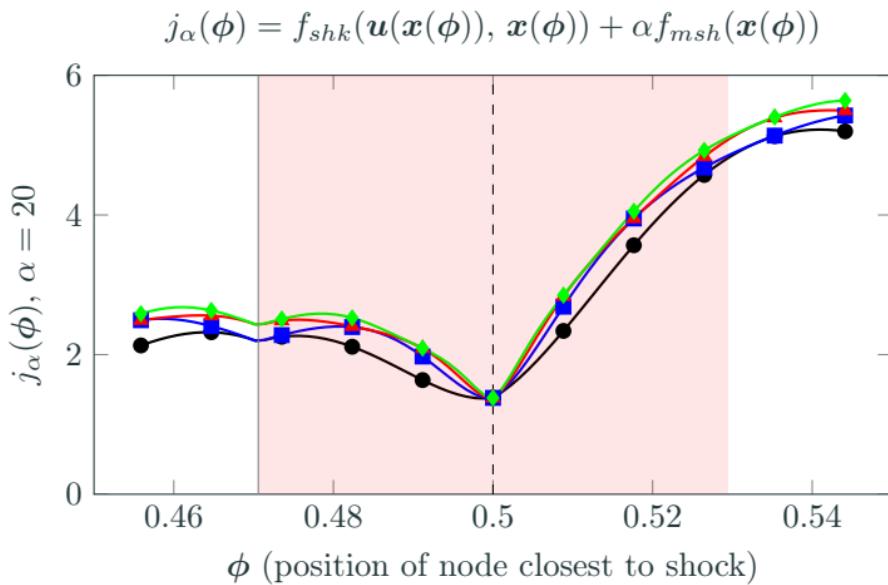
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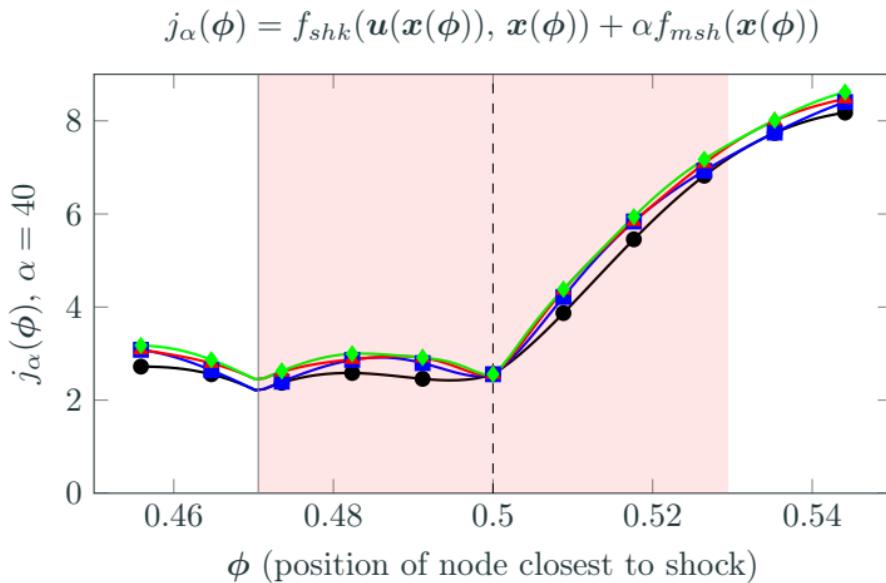
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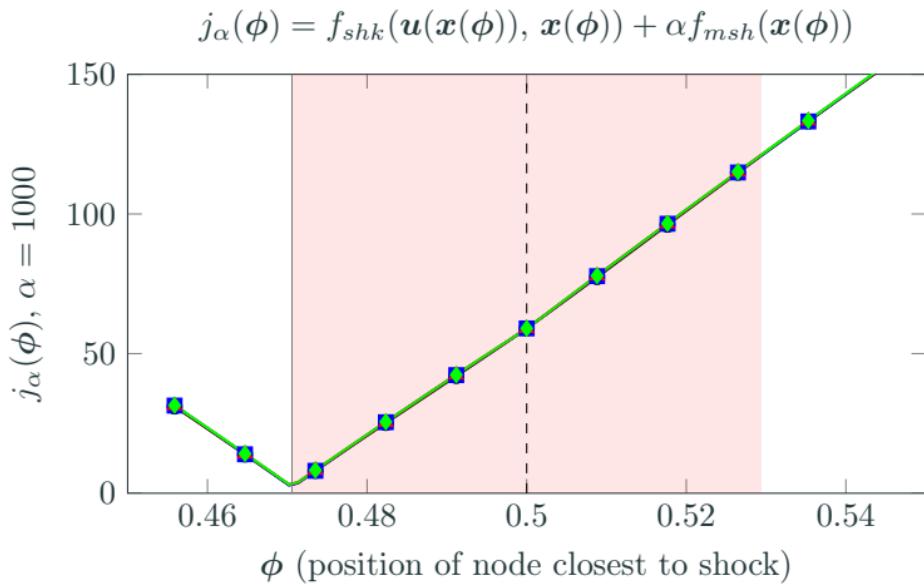
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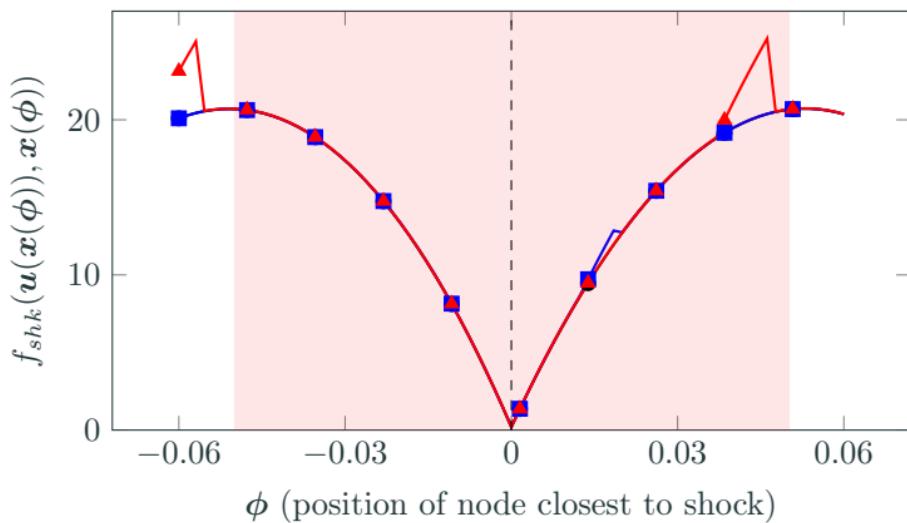
$p = 1$ (●), $p = 2$ (■), $p = 3$ (▲), $p = 4$ (◆).

Objective function monotonically approaches minimum as mesh aligns with discontinuity, regardless of p , for a range of α



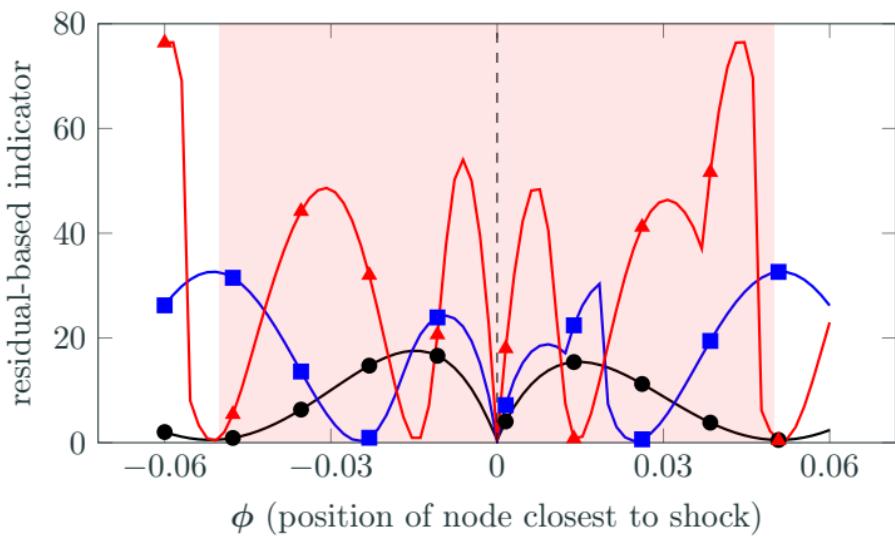
Objective function as an element face is smoothly swept across discontinuity (---):
 $p = 1$ (●), $p = 2$ (■), $p = 3$ (▲), $p = 4$ (◆).

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



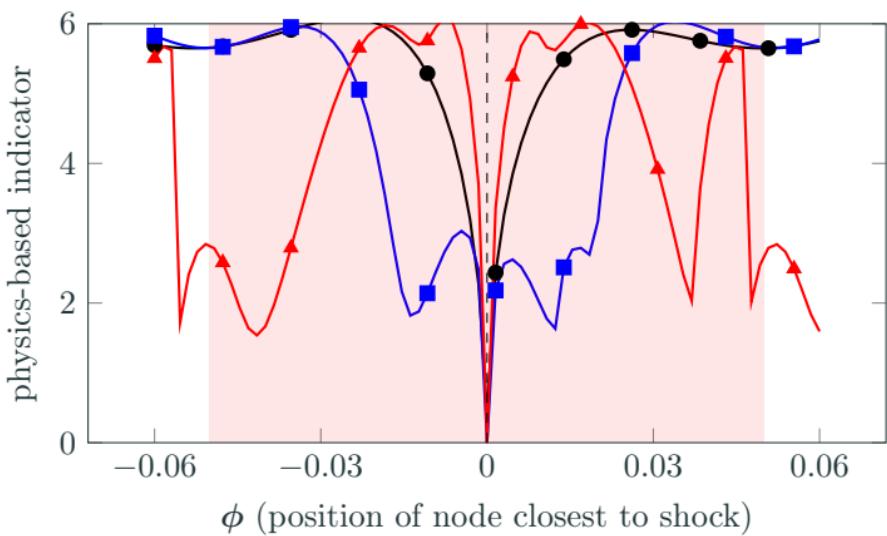
Objective function as an element face is smoothly swept across discontinuity (---):
 $p = 1$ (●—●), $p = 2$ (■—■), $p = 3$ (▲—▲).

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*

¹usually 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 method¹ to solve nonlinear KKT system for $\mathbf{u}^*, \mathbf{x}^*, \boldsymbol{\lambda}^*$

¹usually requires globalization such as linesearch or trust-region

Implementation mostly requires standard terms in implicit code

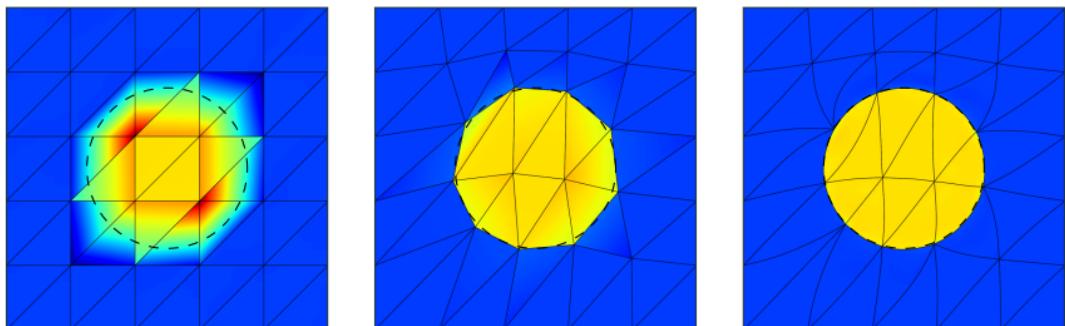
Gradient-based optimizers for the tracking optimization problem will require

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

- \boldsymbol{r} and $\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{u}} \boldsymbol{r}$ required by standard implicit solvers
- Same terms required for reduced space approach

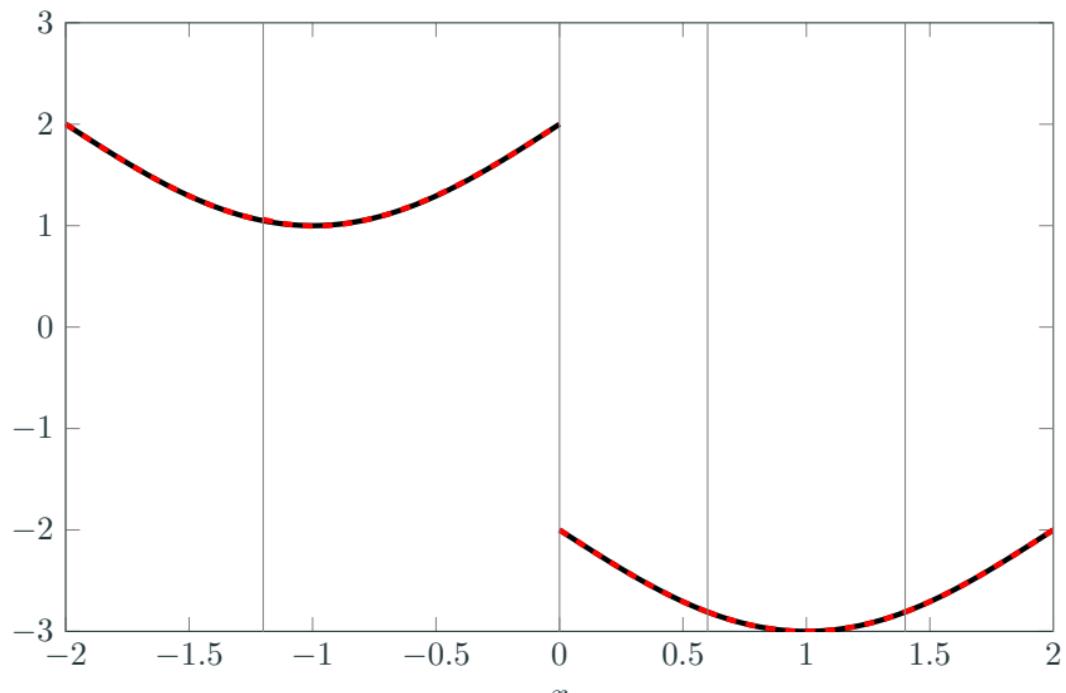
L^2 projection of discontinuous function on DG basis

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



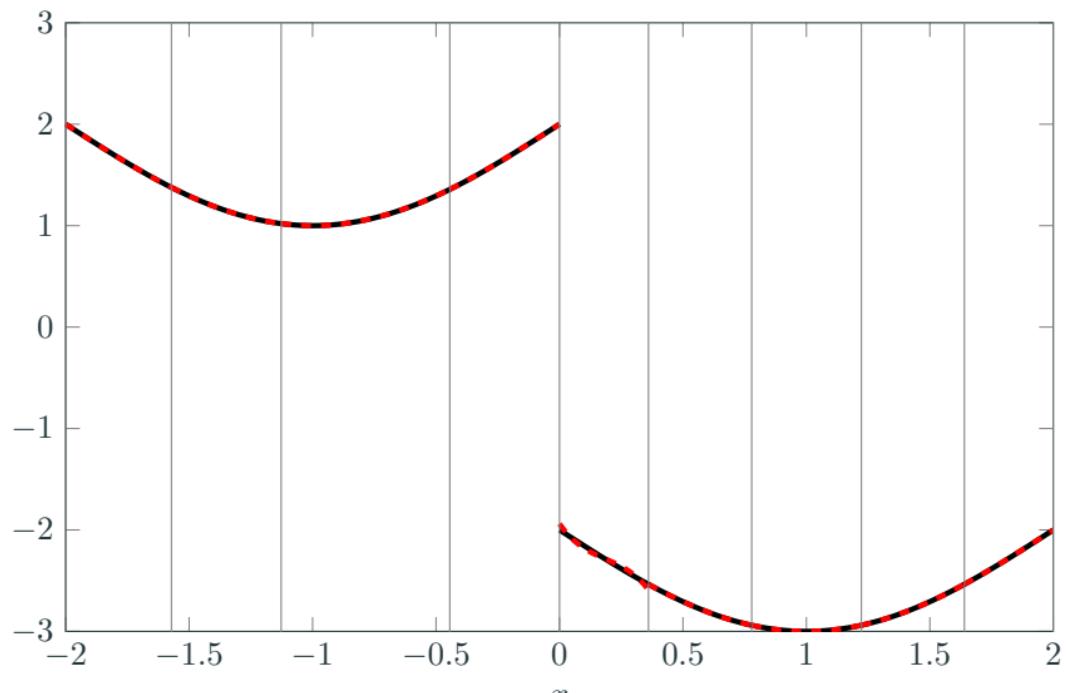
Non-aligned (*left*) vs. discontinuity-aligned mesh with linear (*middle*) and cubic (*right*) elements

Resolution of modified Burgers' equation with few elements



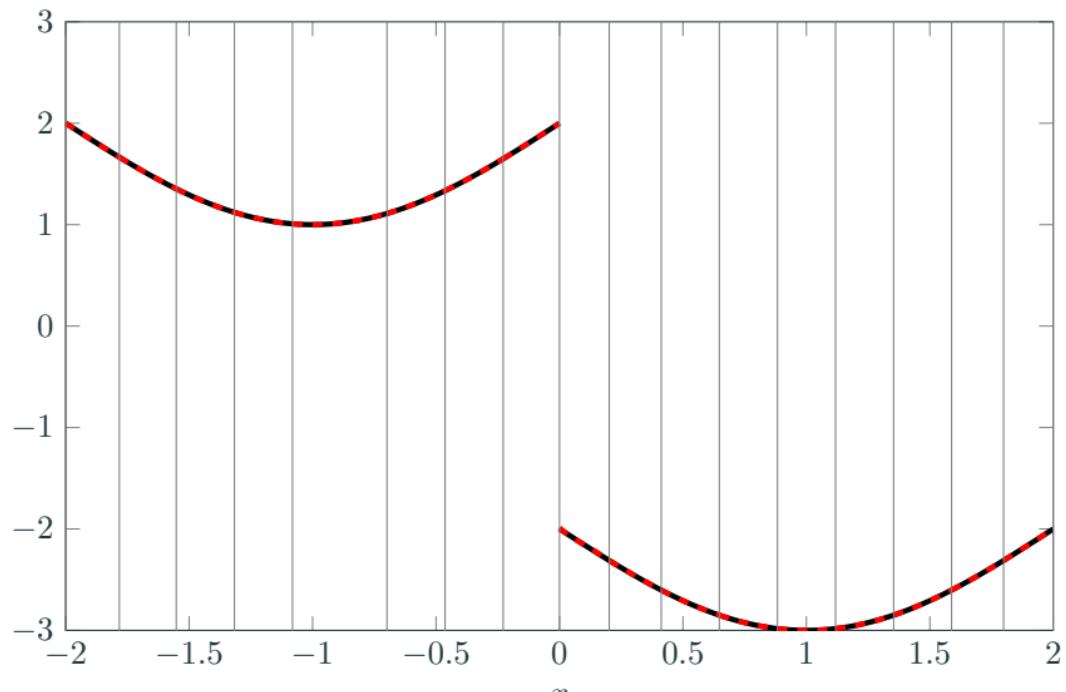
Exact solution (—), tracking solution (---) and mesh (—) for $p = 3$

Resolution of modified Burgers' equation with few elements



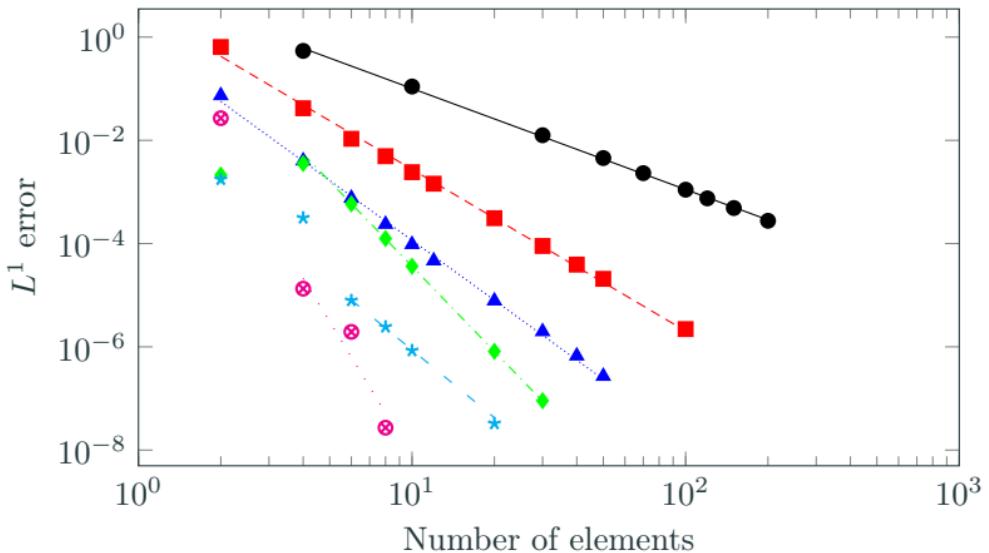
Exact solution (—), tracking solution (---) and mesh (—) for $p = 3$

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

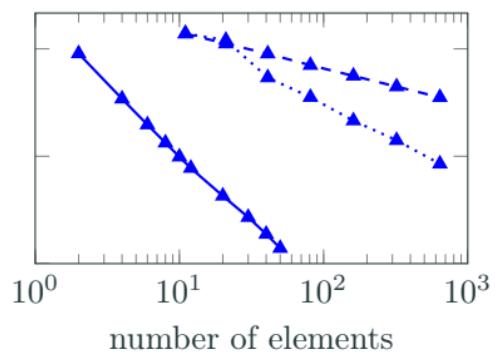
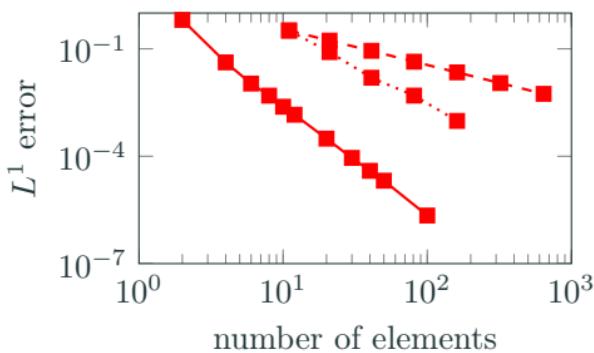
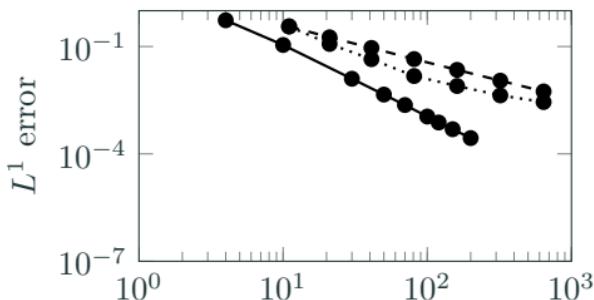


$p = 1$ (\bullet), $p = 2$ (\blacksquare), $p = 3$ (\blacktriangle), $p = 4$ (\blacklozenge), $p = 5$ (\blackstar), $p = 6$ (\textcircled{x})

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

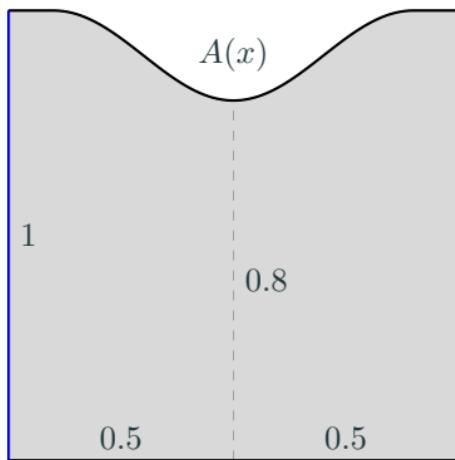
$\angle - 2.0$ (—), $\angle - 3.1$ (— - -), $\angle - 3.9$ (.....), $\angle - 5.5$ (- - -), $\angle - 4.4$ (- - - -), $\angle - 8.7$ (....)

Convergence: tracking vs. uniform/adaptive refinement



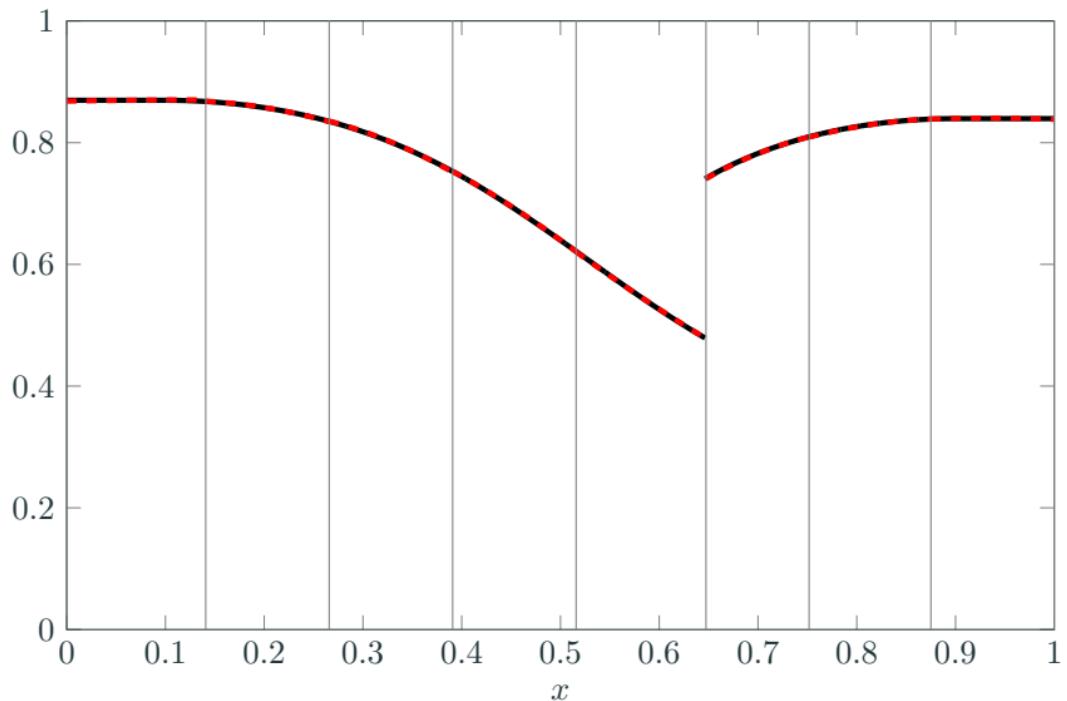
discontinuity-tracking	$p = 1$ (●)	$p = 2$ (■)	$p = 3$ (▲)
uniform refinement	$p = 1$ (-●-)	$p = 2$ (-■-)	$p = 3$ (-▲-)
adaptive refinement	$p = 1$ (··●··)	$p = 2$ (··■··)	$p = 3$ (··▲··)

Nozzle flow: quasi-1d Euler equations



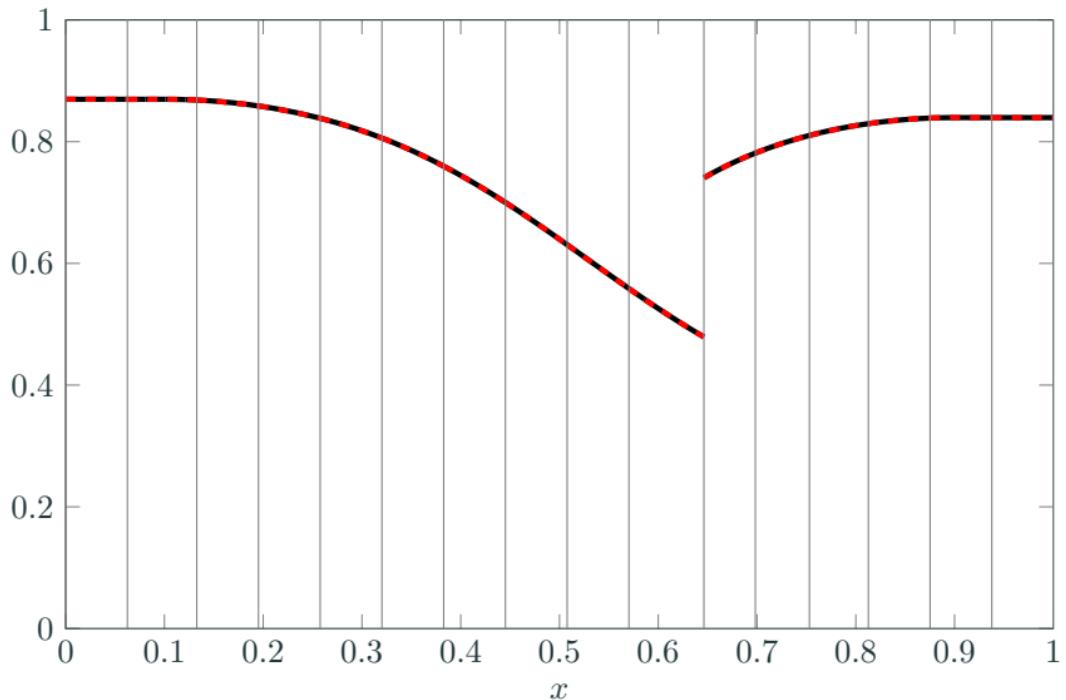
Inviscid wall (—), inflow (—), outflow (—)

Resolution of quasi-1d Euler equations with few elements



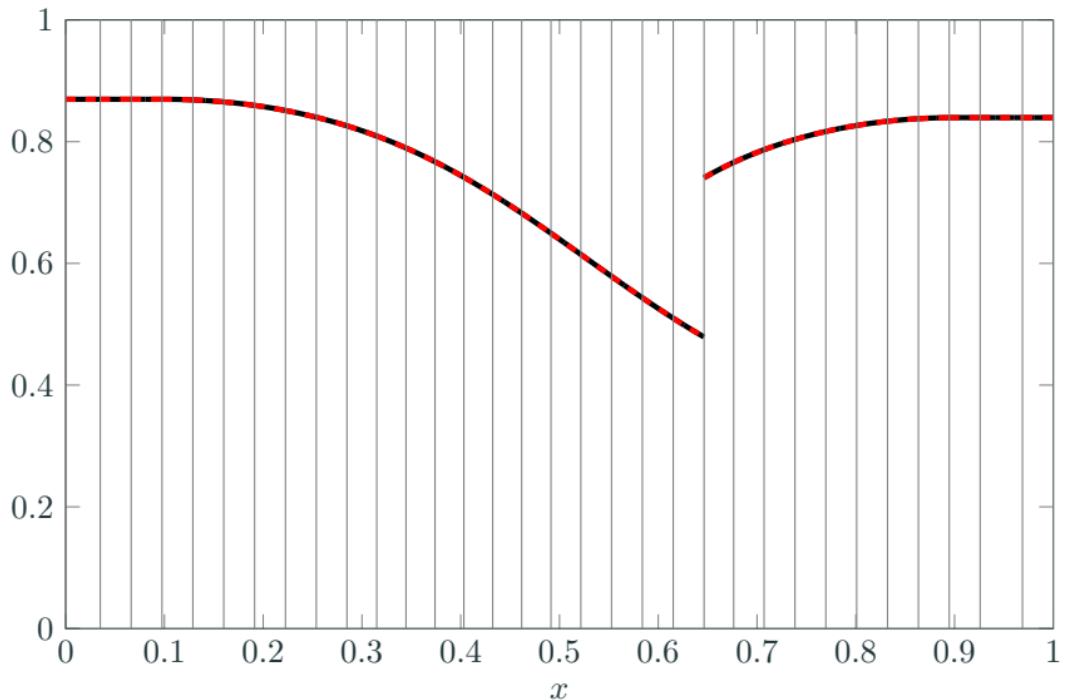
Exact solution (—), tracking solution (- - -) and mesh (—) for $p = 3$

Resolution of quasi-1d Euler equations with few elements



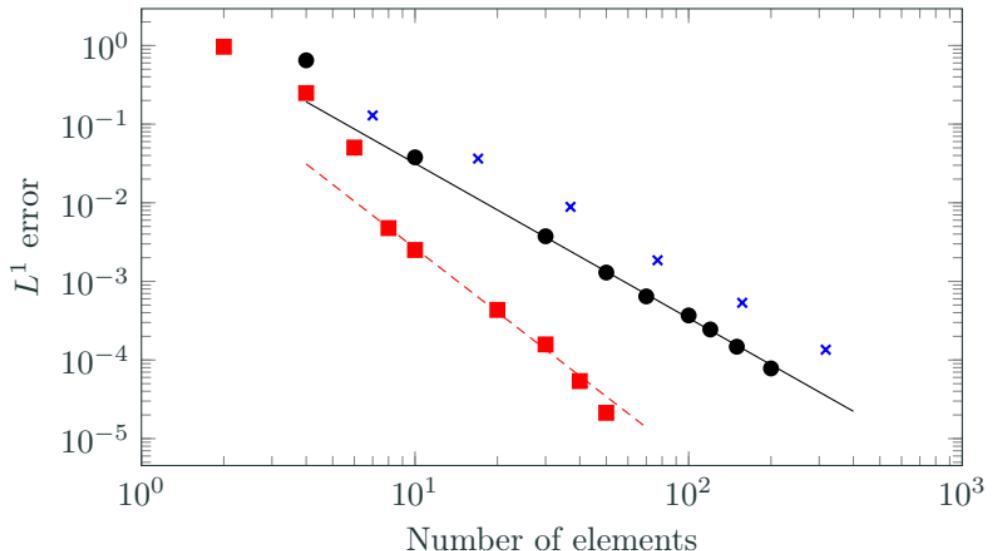
Exact solution (—), tracking solution (- - -) and mesh (—) for $p = 3$

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

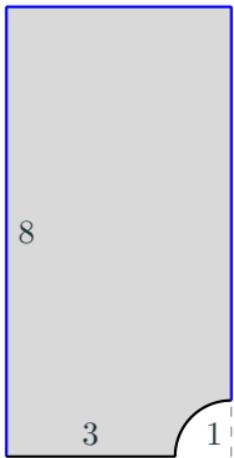


$p = 1$ (●), $p = 2$ (■)

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

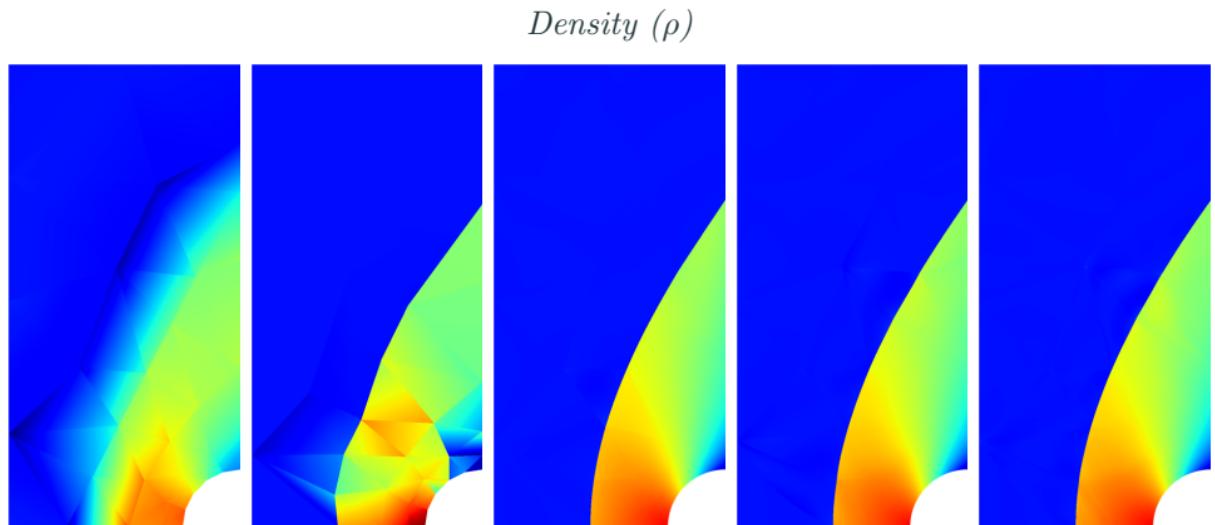
Reference second-order method ($p = 1$) with adaptive mesh refinement (✖)

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



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

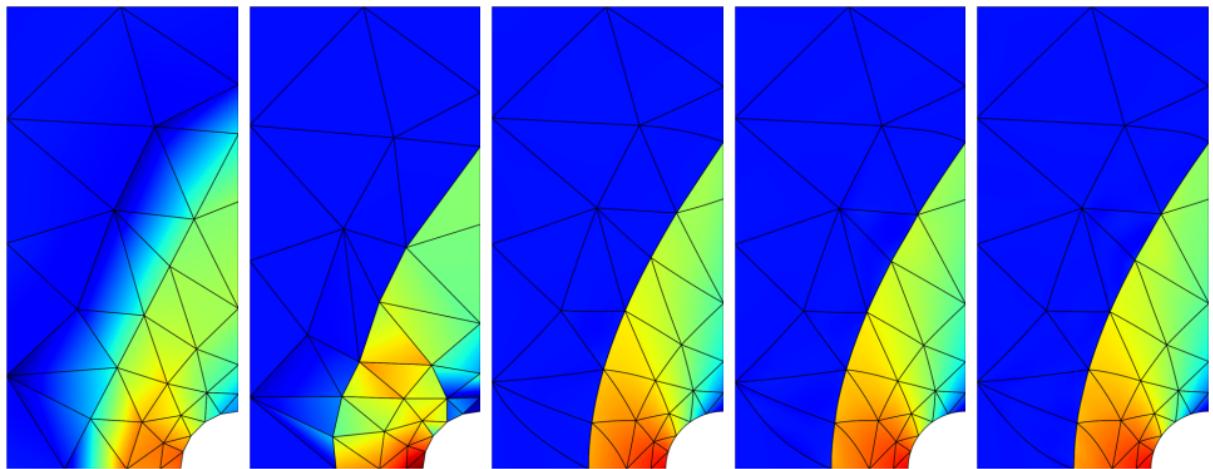
Resolution of 2D supersonic flow with 48 elements



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

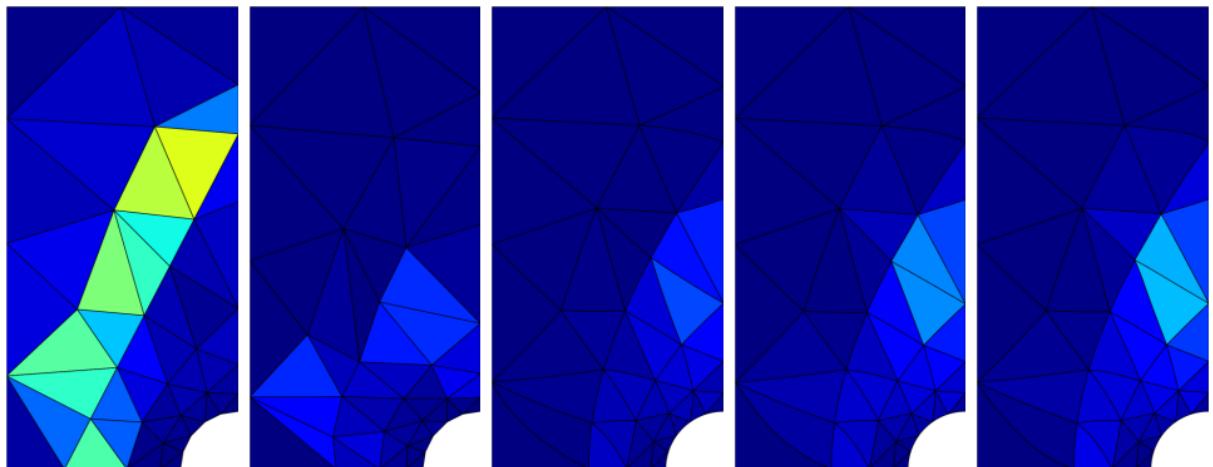
Density (ρ)



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

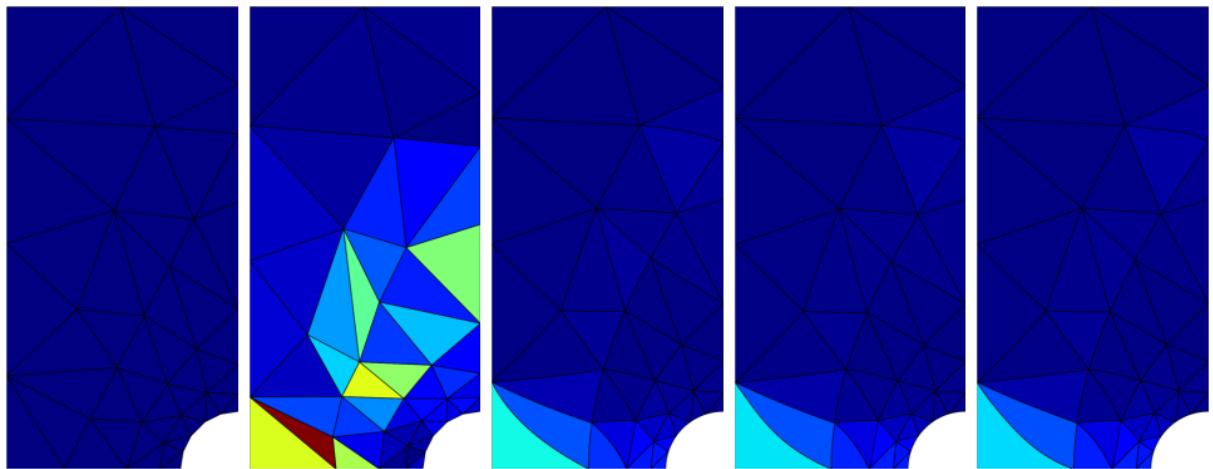
Shock tracking objective (f_{shk})



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})



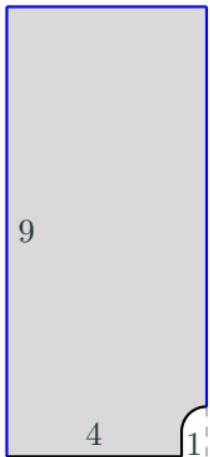
Left: Solution on non-aligned mesh with 48 linear elements and added viscosity (initial guess for shock tracking method). *Remaining:* solution using shock tracking framework corresponding to mesh with 48 $p = 1, p = 2, p = 3, p = 4$ elements.

Convergence to optimal solution and mesh

Discontinuity-tracking performance summary

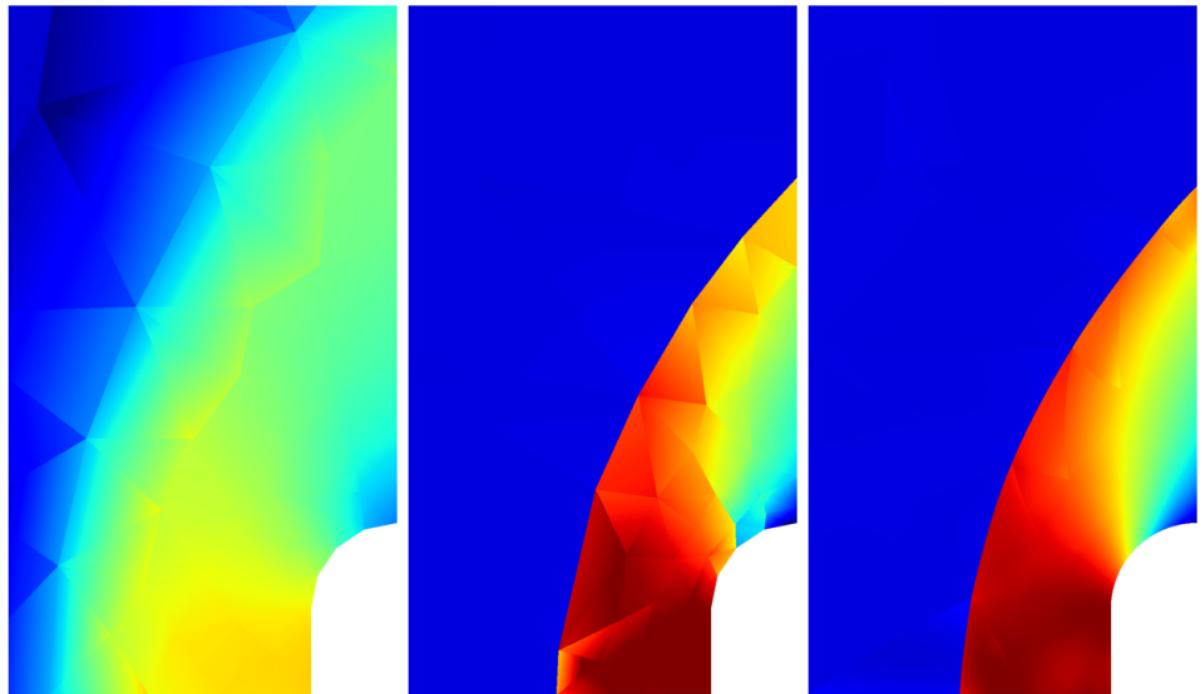
Polynomial order (p)	1	2	3	4
Degrees of freedom ($N_{\mathbf{u}}$)	576	1152	1920	2880
Enthalpy error (e_H)	0.0106	0.000462	0.00151	0.000885
Stagnation pressure error (e_p)	0.0711	0.00479	0.0112	0.000616

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



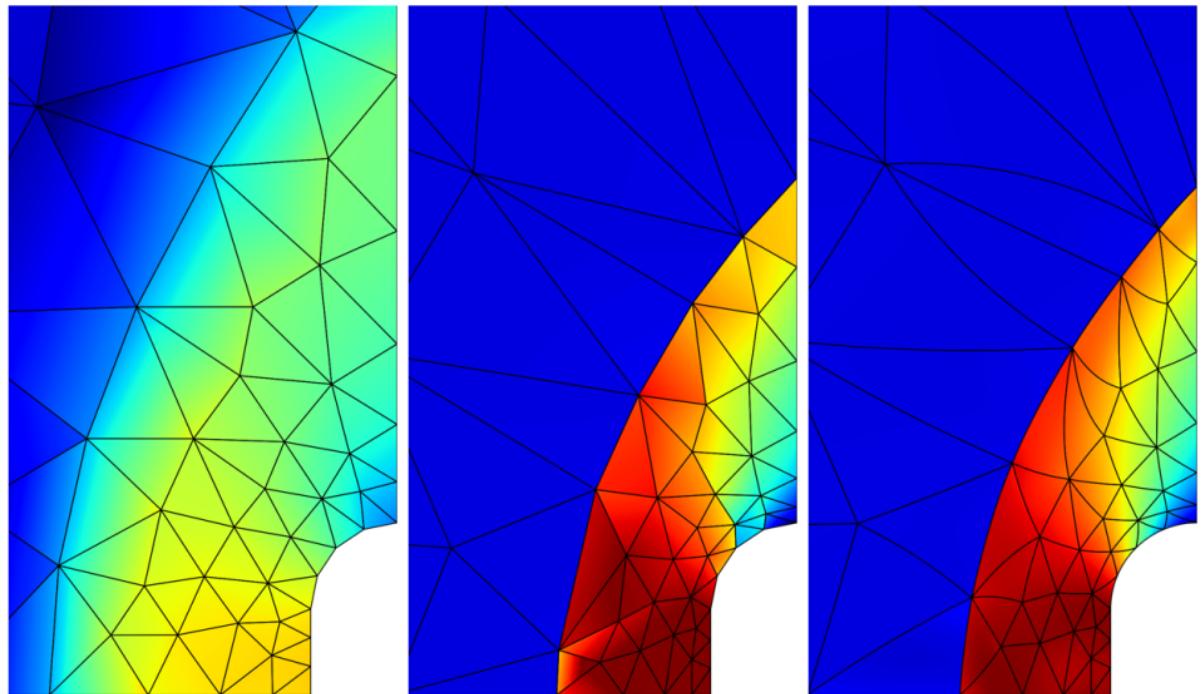
Inviscid wall/symmetry condition (—) and farfield (—)

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.

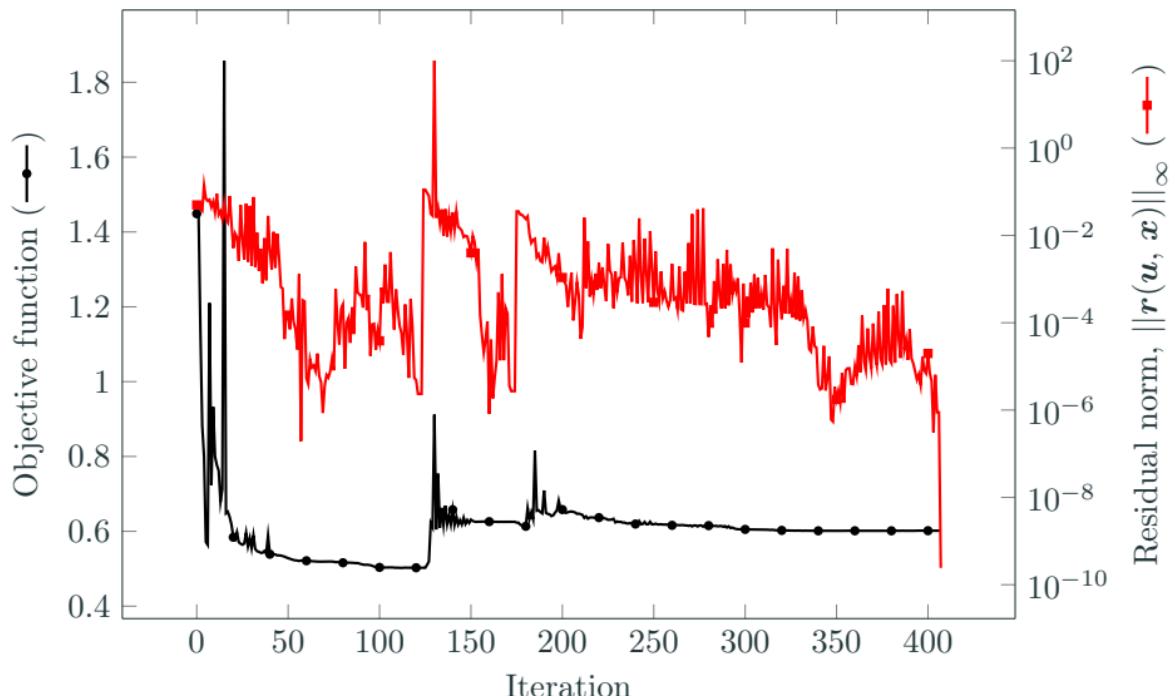
Resolution of 2D supersonic flow with 102 quadratic elements



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.

Convergence to optimal solution and mesh

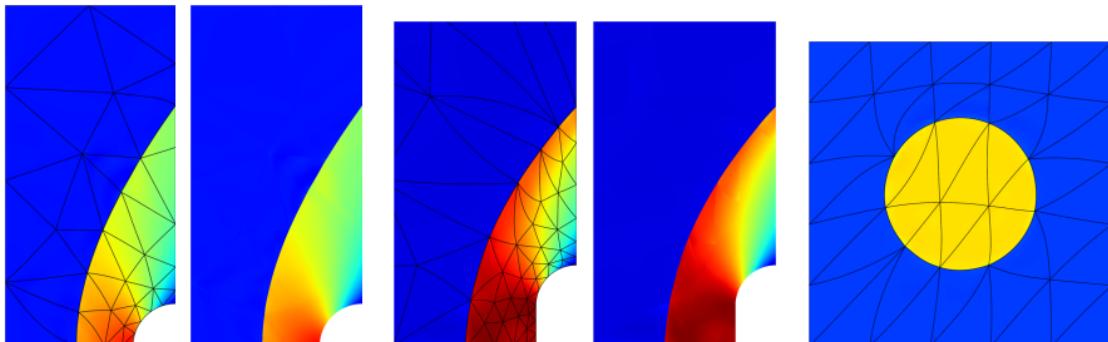
Solver simultaneously minimizes objective and solves PDE



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*).

References I

-  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).
Energetically optimal flapping flight based on a fully discrete adjoint method with explicit treatment of flapping frequency.
In *Proc. of the 23rd AIAA Computational Fluid Dynamics Conference*, Denver, Colorado. American Institute of Aeronautics and Astronautics.

References II

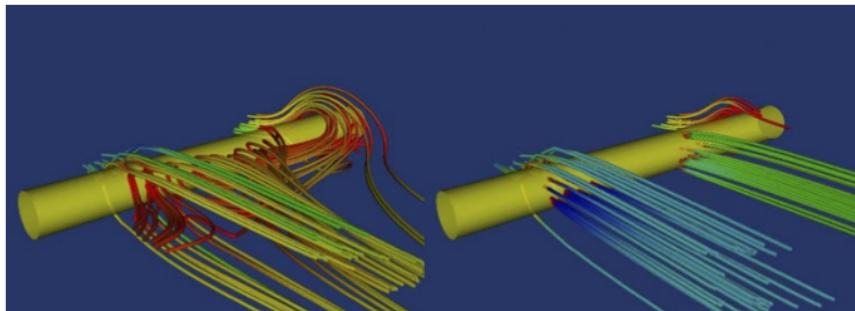
-  Zahr, M. J. and Persson, P.-O. (1/8/2018 – 1/12/2018b).
An optimization-based discontinuous Galerkin approach for high-order accurate shock tracking.
In *AIAA Science and Technology Forum and Exposition (SciTech2018)*, Kissimmee, Florida. American Institute of Aeronautics and Astronautics.
-  Zahr, M. J. and Persson, P.-O. (2016).
An adjoint method for a high-order discretization of deforming domain conservation laws for optimization of flow problems.
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.

References III

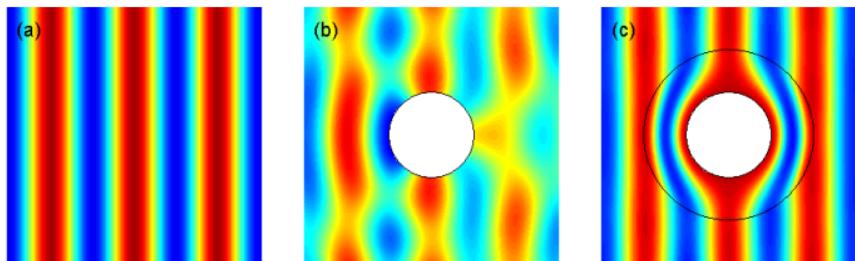
-  Zahr, M. J., Persson, P.-O., and Wilkening, J. (2016).
A fully discrete adjoint method for optimization of flow problems on deforming domains with time-periodicity constraints.
Computers & Fluids, 139:130 – 147.

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

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

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

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

- *Fully discrete* PDE-constrained optimization problem

$$\begin{array}{ll} \underset{\substack{\boldsymbol{u}_0, \dots, \boldsymbol{u}_{N_t} \in \mathbb{R}^{N_u}, \\ \boldsymbol{k}_{1,1}, \dots, \boldsymbol{k}_{N_t,s} \in \mathbb{R}^{N_u}, \\ \boldsymbol{\mu} \in \mathbb{R}^{n_\mu}}}{\text{minimize}} & J(\boldsymbol{u}_0, \dots, \boldsymbol{u}_{N_t}, \boldsymbol{k}_{1,1}, \dots, \boldsymbol{k}_{N_t,s}, \boldsymbol{\mu}) \end{array}$$

$$\text{subject to} \quad \mathbf{C}(\boldsymbol{u}_0, \dots, \boldsymbol{u}_{N_t}, \boldsymbol{k}_{1,1}, \dots, \boldsymbol{k}_{N_t,s}, \boldsymbol{\mu}) \leq 0$$

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

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

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

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

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

$$r(\mu) = r(u(\mu), \mu) = 0, \quad F(\mu) = F(u(\mu), \mu)$$

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

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

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

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

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

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

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

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

The total derivative of F

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

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

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

The total derivative of F

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

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

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

The total derivative of F

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

Algebraic equations leads to adjoint equations

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

Sensitivity vs. adjoint method to compute gradient of F

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

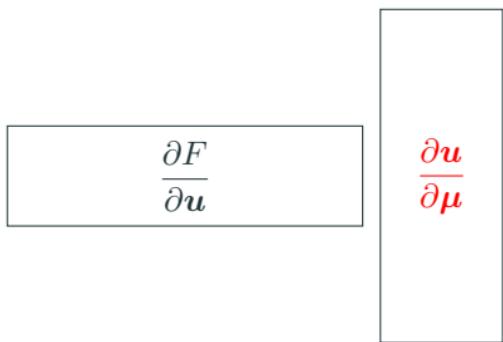
$$\frac{\partial F}{\partial u}$$

$$\frac{\partial r}{\partial u}^{-1}$$

$$\frac{\partial r}{\partial \mu}$$

Sensitivity vs. adjoint method to compute gradient of F

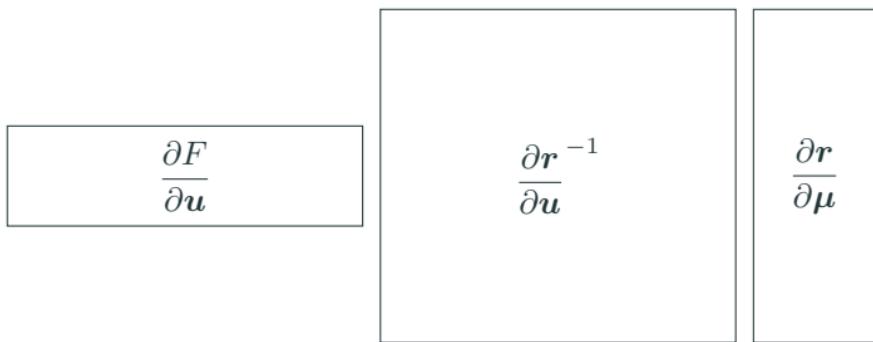
$$\frac{\partial F}{\partial \boldsymbol{u}} \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{u}}^{-1} \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{\mu}}$$



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

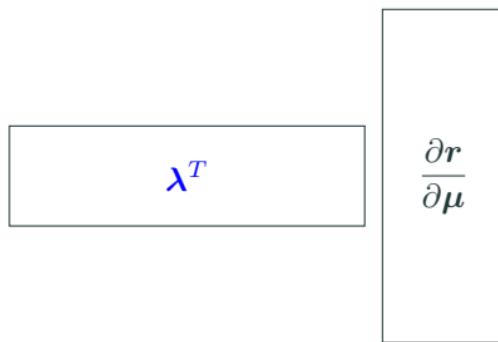
$$\frac{\partial F}{\partial \boldsymbol{u}} \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{u}}^{-1} \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{\mu}}$$



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

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



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

$$\underset{\substack{\boldsymbol{u}_0, \dots, \boldsymbol{u}_{N_t} \in \mathbb{R}^{N_u}, \\ \boldsymbol{k}_{1,1}, \dots, \boldsymbol{k}_{N_t,s} \in \mathbb{R}^{N_u}}}{\text{minimize}} \quad F(\boldsymbol{u}_0, \dots, \boldsymbol{u}_{N_t}, \boldsymbol{k}_{1,1}, \dots, \boldsymbol{k}_{N_t,s}, \boldsymbol{\mu})$$

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

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

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

- Define **Lagrangian**

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

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

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

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

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

Reconstructed flow

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

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

Reconstructed flow

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

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

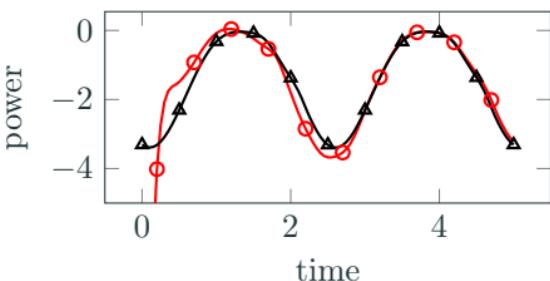
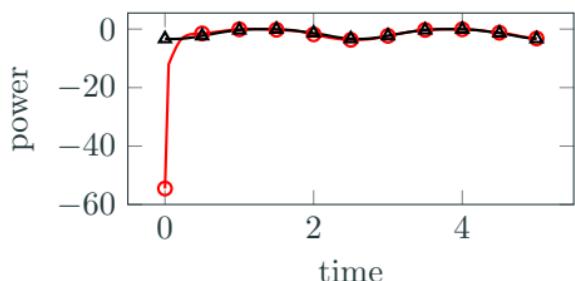
subject to $\boldsymbol{U}(\boldsymbol{x}, 0) = \boldsymbol{U}(\boldsymbol{x}, T)$

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

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

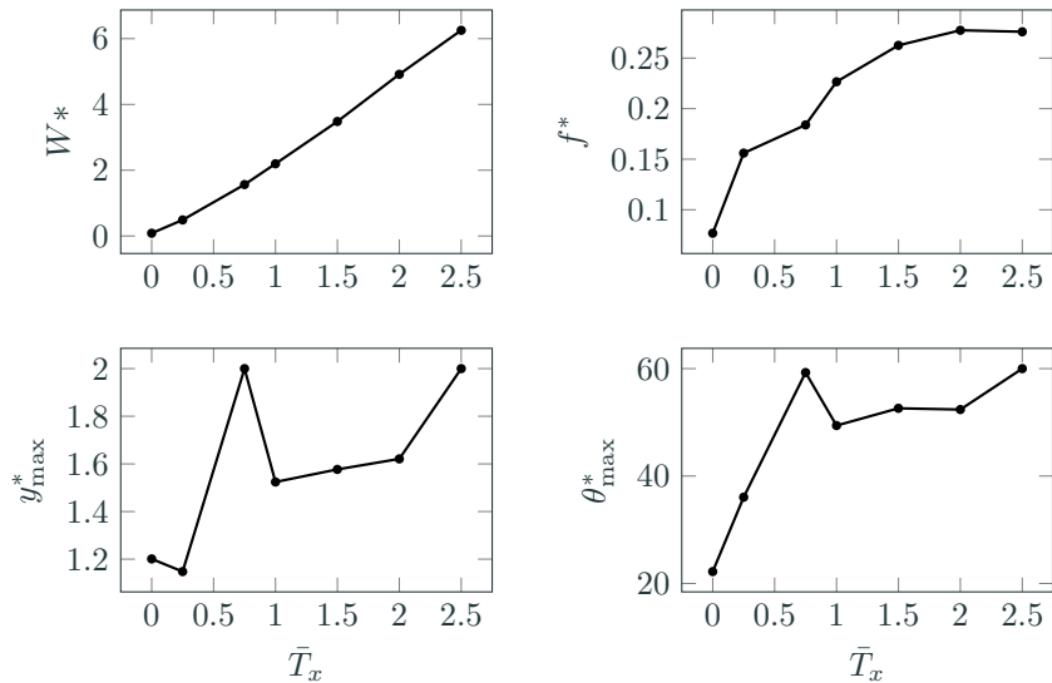
$$\boldsymbol{\lambda}_{n-1} = \boldsymbol{\lambda}_n + \frac{\partial F}{\partial \boldsymbol{u}_{n-1}}^T + \sum_{i=1}^s \Delta t_n \frac{\partial \boldsymbol{r}_{n,i}}{\partial \boldsymbol{u}}^T \boldsymbol{\kappa}_{n,i}$$

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



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

Energetically optimal flapping vs. required thrust: QoI



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

Initial guess for optimization: \mathbf{u}_0 , ϕ_0

- Initial guess for \mathbf{u} and ϕ 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:
 - ϕ_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 ν

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

Modified Burgers' equation with discontinuous source term

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

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

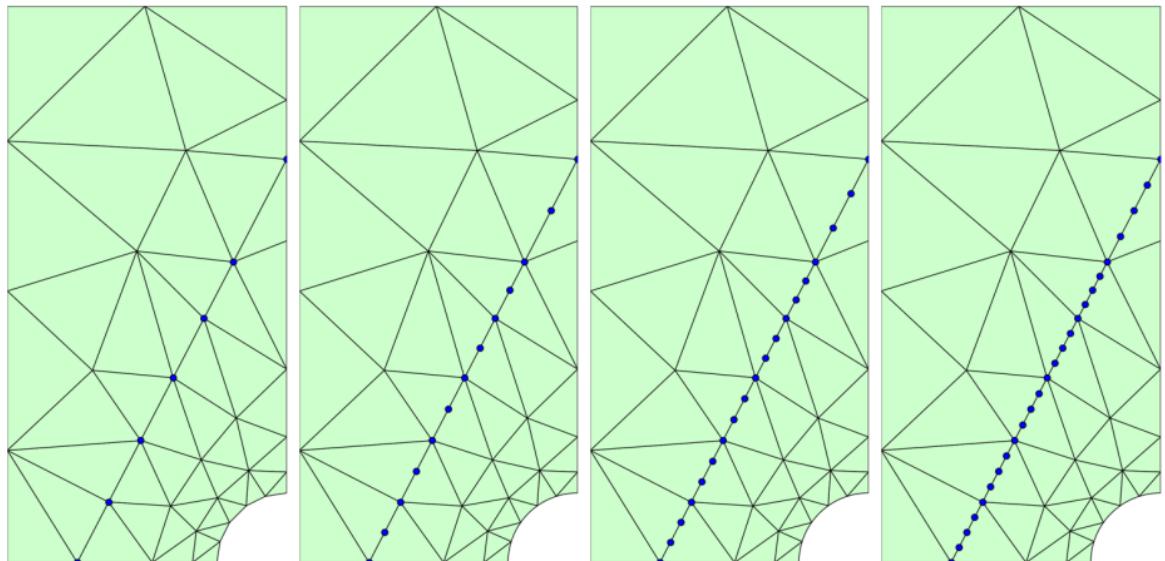
where $u(-2) = 2$, $u(2) = -2$, $\beta = -0.1$ and

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

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.