

A robust, high-order implicit shock tracking method for high-speed flows

Matthew J. Zahr

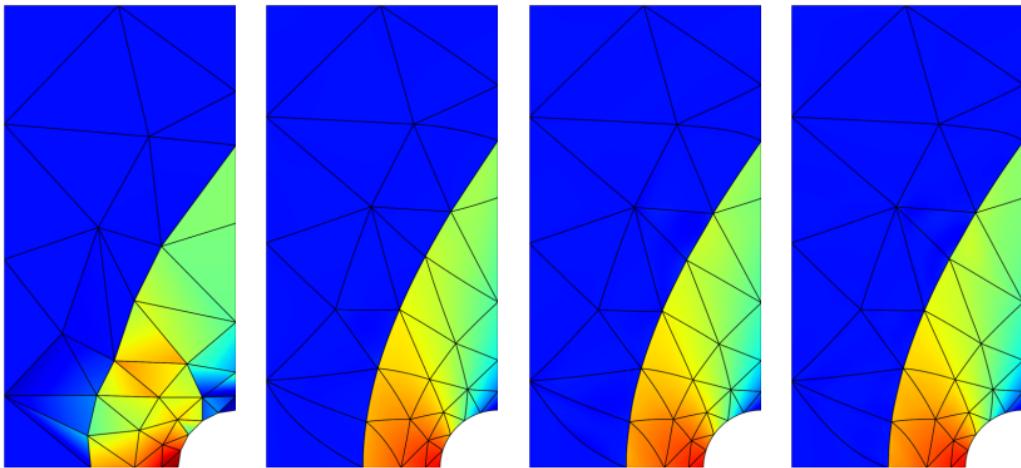
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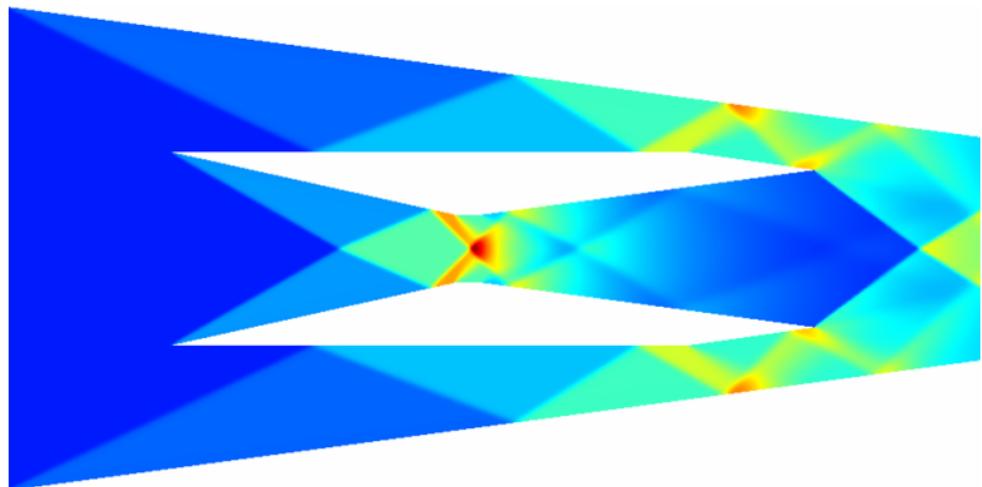
Why high-order tracking: Accurate solutions on coarse meshes



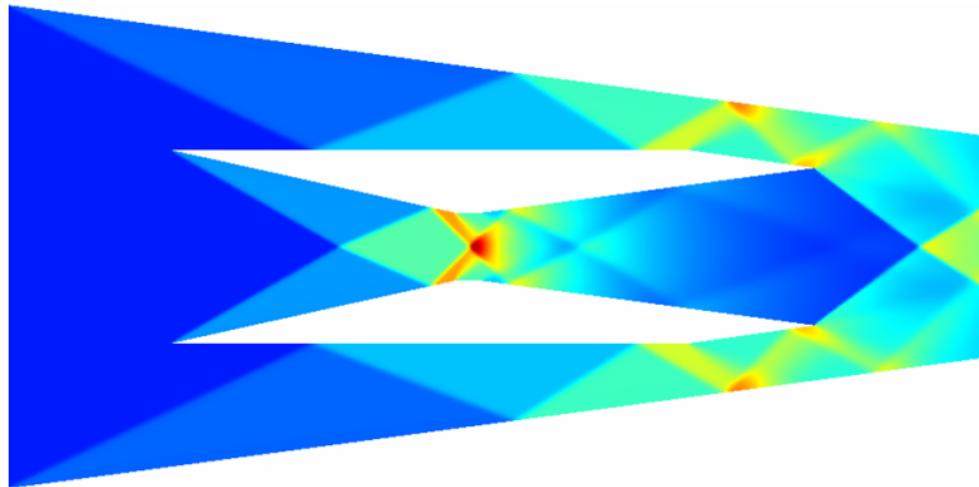
Density of supersonic flow ($M = 2$) past a cylinder using implicit shock tracking with $p = 1$ to $p = 4$ (left to right) DG discretization.

Key observation: High-order tracking enables accurate resolution of 2D supersonic flow with 48 elements; the error in the stagnation enthalpy is $\mathcal{O}(10^{-4})$ for $p = 2$ (1152 DoF).

Why not tracking: Difficult for complex discontinuity surfaces



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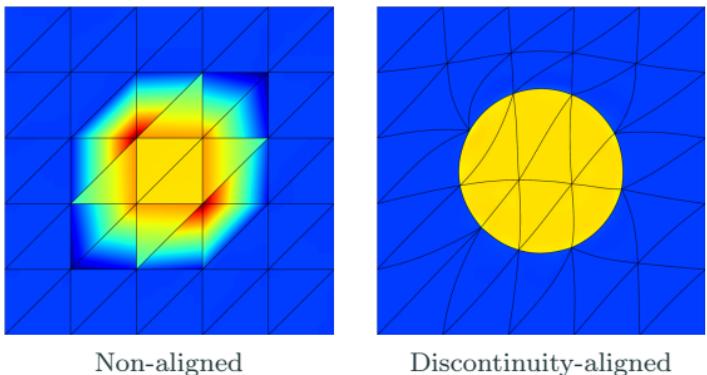


Implicit shock tracking

Aims to overcome the difficulty of explicitly meshing the unknown shock surface, e.g., HOIST [Zahr, Persson; 2018], MDG-ICE [Corrigan, Kercher, Kessler; 2019]

Implicit tracking 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



High-order implicit shock tracking (HOIST)¹

- Discontinuous Galerkin discretization: inter-element jumps, high-order
- Discontinuity-aligned mesh: solution of optimization problem constrained by the discrete PDE \implies **implicit tracking**
- Full space solver that converges the solution and mesh simultaneously to ensure solution of PDE never required on non-aligned mesh

¹[Zahr, Persson; 2018], [Zahr, Shi, Persson; 2020]

Discontinuous Galerkin discretization of conservation law

Inviscid conservation law:

$$\nabla \cdot F(U) = 0 \quad \text{in } \Omega$$

Element-wise finite-dimensional weak form of conservation law:

$$r_{h,p'}^K(U_{h,p}) := \int_{\partial K} \psi_{h,p'}^+ \cdot \mathcal{H}(U_{h,p}^+, U_{h,p}^-, n) dS - \int_K F(U_{h,p}) : \nabla \psi_{h,p'} dV,$$

where $\mathcal{V}_{h,p'}$ is the test space, $\mathcal{V}_{h,p}$ is the trial space, \mathcal{H} is the numerical flux function, h is element size, and p/p' is the polynomial degree.

Introduce basis for polynomial spaces to obtain discrete residuals

$$\mathbf{r}(\mathbf{u}, \mathbf{x}) \quad (p' = p), \quad \mathbf{R}(\mathbf{u}, \mathbf{x}) \quad (p' = p + 1),$$

where \mathbf{u} is the discrete state vector and \mathbf{x} are the coordinates of the mesh nodes.

Implicit shock tracking: constrained optimization formulation

We formulate the problem of tracking discontinuities with the mesh as the solution of an optimization problem constrained by the discrete PDE (DG discretization)

$$\begin{aligned} & \underset{\boldsymbol{u}, \boldsymbol{x}}{\text{minimize}} \quad f(\boldsymbol{u}, \boldsymbol{x}) := \frac{1}{2} \|\boldsymbol{F}(\boldsymbol{u}, \boldsymbol{x})\|_2^2 \\ & \text{subject to} \quad \boldsymbol{r}(\boldsymbol{u}, \boldsymbol{x}) = \mathbf{0}. \end{aligned}$$

The objective function *balances* tracking and mesh quality

$$\boldsymbol{F}(\boldsymbol{u}, \boldsymbol{x}) = \begin{bmatrix} \boldsymbol{R}(\boldsymbol{u}, \boldsymbol{x}) \\ \kappa \boldsymbol{R}_{\text{msh}}(\boldsymbol{x}) \end{bmatrix}$$

$\boldsymbol{r}(\boldsymbol{u}, \boldsymbol{x}) = \mathbf{0}$ (DG equation), \boldsymbol{u} (discrete state vector), \boldsymbol{x} (coordinates of mesh nodes)

\boldsymbol{R} (tracking term): penalizes the DG residual in the *enriched test space*

$\boldsymbol{R}_{\text{msh}}$ (mesh term): accounts for the distortion of each high-order element

κ : mesh distortion penalization parameter

Implicit shock tracking: sequential quadratic programming solver

Define $\mathbf{z} = (\mathbf{u}, \mathbf{x})$ and use interchangeably. To solve the optimization problem, we define a sequence $\{\mathbf{z}_k\}$ updated as

$$\mathbf{z}_{k+1} = \mathbf{z}_k + \alpha_k \Delta \mathbf{z}_k.$$

Implicit shock tracking: sequential quadratic programming solver

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$$\mathbf{z}_{k+1} = \mathbf{z}_k + \alpha_k \Delta \mathbf{z}_k.$$

The step direction $\Delta \mathbf{z}_k$ is defined as the solution of the quadratic program (QP) approximation of the tracking problem centered at \mathbf{z}_k

$$\begin{aligned} & \underset{\Delta \mathbf{z} \in \mathbb{R}^{N_z}}{\text{minimize}} \quad \mathbf{g}_z(\mathbf{z}_k)^T \Delta \mathbf{z} + \frac{1}{2} \Delta \mathbf{z}^T \mathbf{B}_z(\mathbf{z}_k, \hat{\boldsymbol{\lambda}}(\mathbf{z}_k)) \Delta \mathbf{z} \\ & \text{subject to} \quad \mathbf{r}(\mathbf{z}_k) + \mathbf{J}_z(\mathbf{z}_k) \Delta \mathbf{z} = \mathbf{0}, \end{aligned}$$

where

$$\mathbf{g}_z(z) = \frac{\partial f}{\partial z}(z)^T, \quad \mathbf{J}_z(z) = \frac{\partial \mathbf{r}}{\partial z}(z), \quad \mathbf{B}_z(z, \boldsymbol{\lambda}) \approx \frac{\partial^2 \mathcal{L}}{\partial z \partial z}(z, \boldsymbol{\lambda}),$$

$$\mathcal{L}(z, \boldsymbol{\lambda}) = f(z) - \boldsymbol{\lambda}^T \mathbf{r}(z) \quad (\text{Lagrangian})$$

$$\hat{\boldsymbol{\lambda}}(z) = \frac{\partial \mathbf{r}}{\partial \mathbf{u}}(z)^{-T} \frac{\partial f}{\partial \mathbf{u}}(z)^T \quad (\text{Lagrange multiplier estimate})$$

Implicit shock tracking: sequential quadratic programming solver

The solution of the quadratic program leads to the following linear system

$$\begin{bmatrix} B_{uu}(z_k, \hat{\lambda}(z_k)) & B_{ux}(z_k, \hat{\lambda}(z_k)) & J_u(z_k)^T \\ B_{ux}(z_k, \hat{\lambda}(z_k))^T & B_{xx}(z_k, \hat{\lambda}(z_k)) & J_x(z_k)^T \\ J_u(z_k) & J_x(z_k) & 0 \end{bmatrix} \begin{bmatrix} \Delta u_k \\ \Delta x_k \\ \eta_k \end{bmatrix} = - \begin{bmatrix} g_u(z_k) \\ g_x(z_k) \\ r(z_k) \end{bmatrix},$$

where

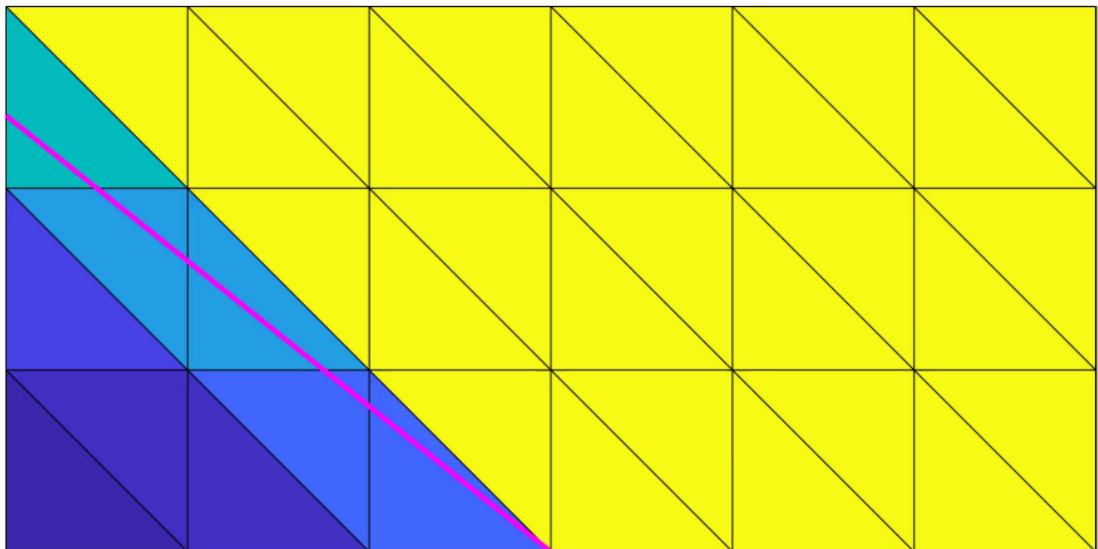
$$g_u(z) = \frac{\partial f}{\partial u}(z)^T, \quad J_u(z) = \frac{\partial r}{\partial u}(z), \quad g_x(z) = \frac{\partial f}{\partial x}(z)^T, \quad J_x(z) = \frac{\partial r}{\partial x}(z),$$

the approximate Hessian of the Lagrangian is taken as

$$\begin{aligned} B_{uu}(z, \lambda) &= \frac{\partial F}{\partial u}(z)^T \frac{\partial F}{\partial u}(z), & B_{ux}(z, \lambda) &= \frac{\partial F}{\partial u}(z)^T \frac{\partial F}{\partial x}(z), \\ B_{xx}(z, \lambda) &= \frac{\partial F}{\partial x}(z)^T \frac{\partial F}{\partial x}(z) + \gamma D, \end{aligned}$$

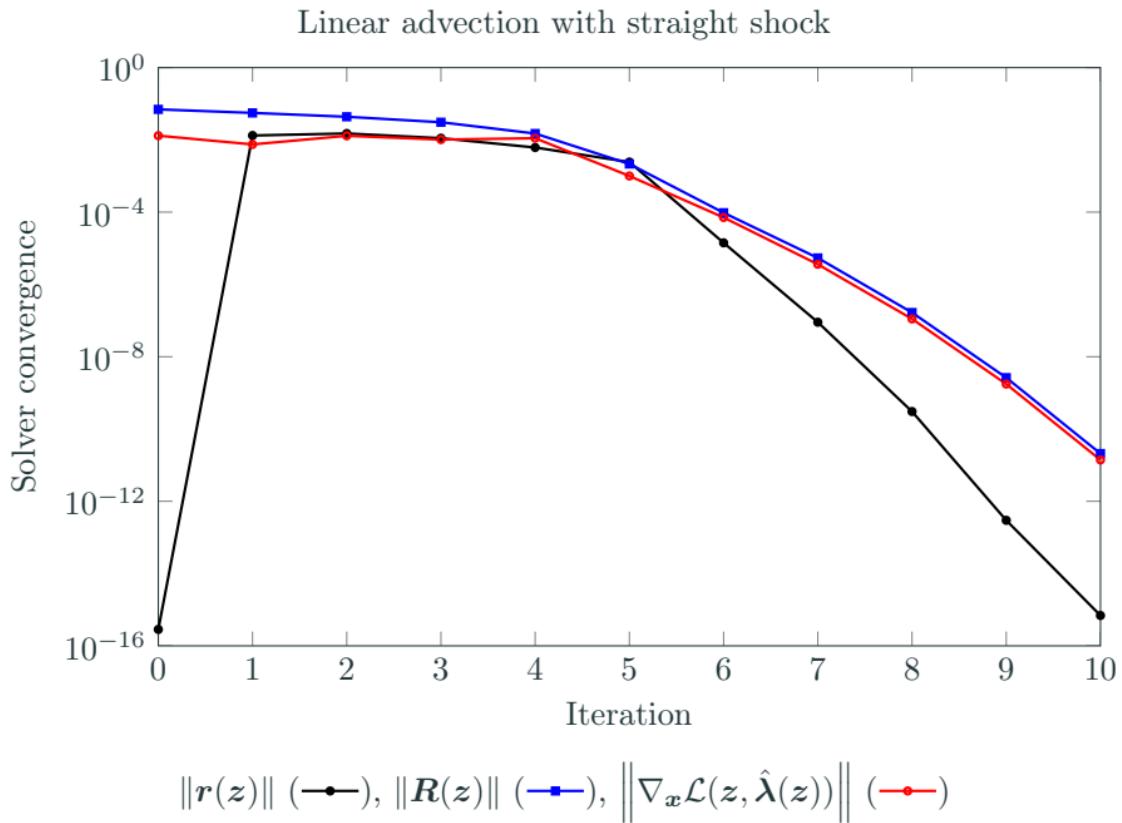
and η_k are the Lagrange multipliers of the QP and D is a mesh regularization matrix (linear elasticity stiffness).

Linear advection (2D), straight shock

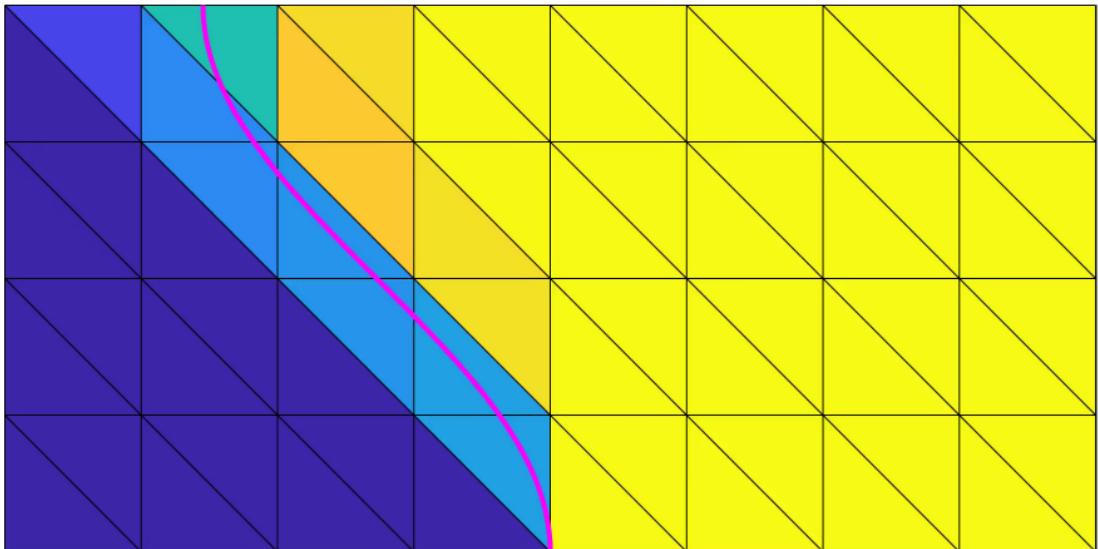


$p = 0$ space for solution, $q = 1$ space for mesh

Newton-like convergence when solution lies in DG subspace

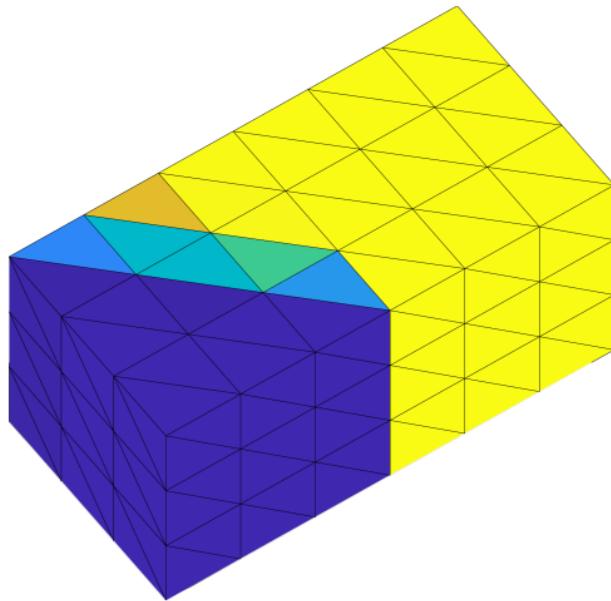


Linear advection (2D), trigonometric shock



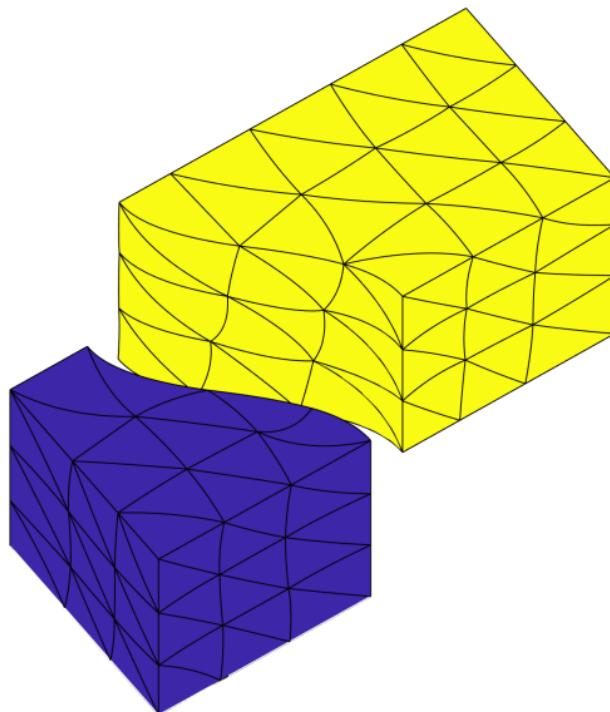
$p = 0$ space for solution, $q = 2$ space for mesh

Linear advection (3D), trigonometric shock



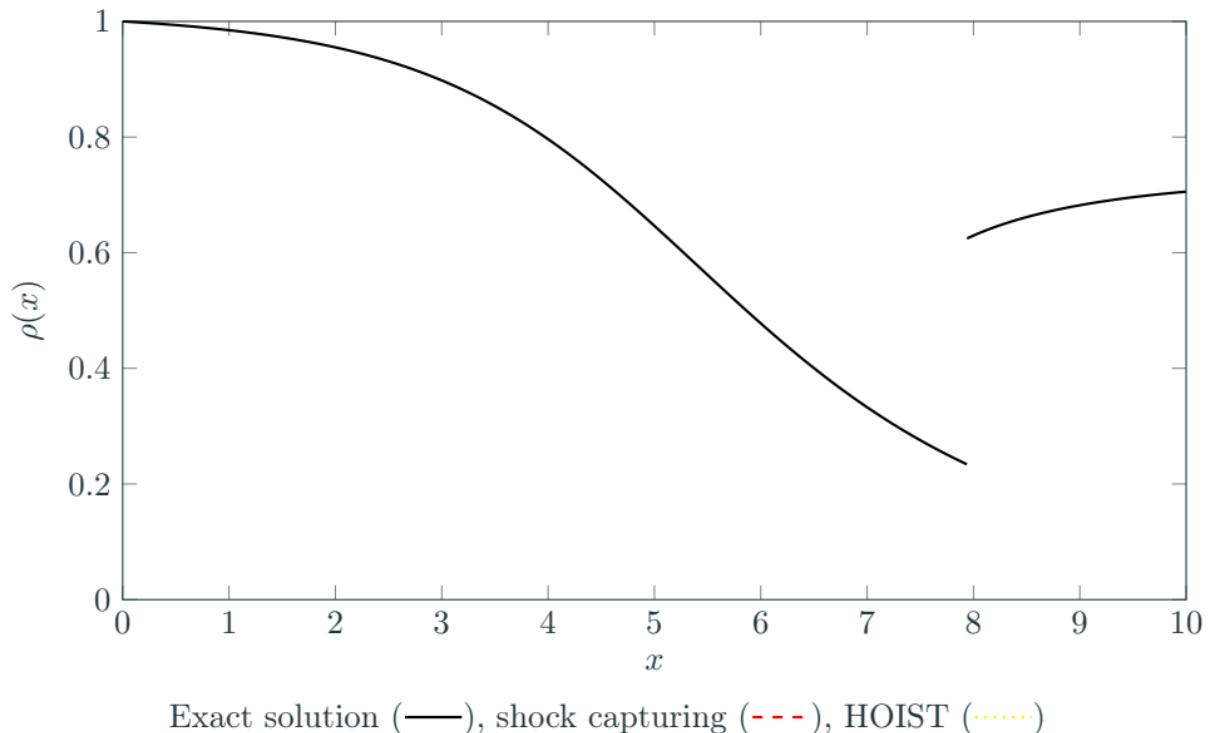
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Linear advection (3D), trigonometric shock

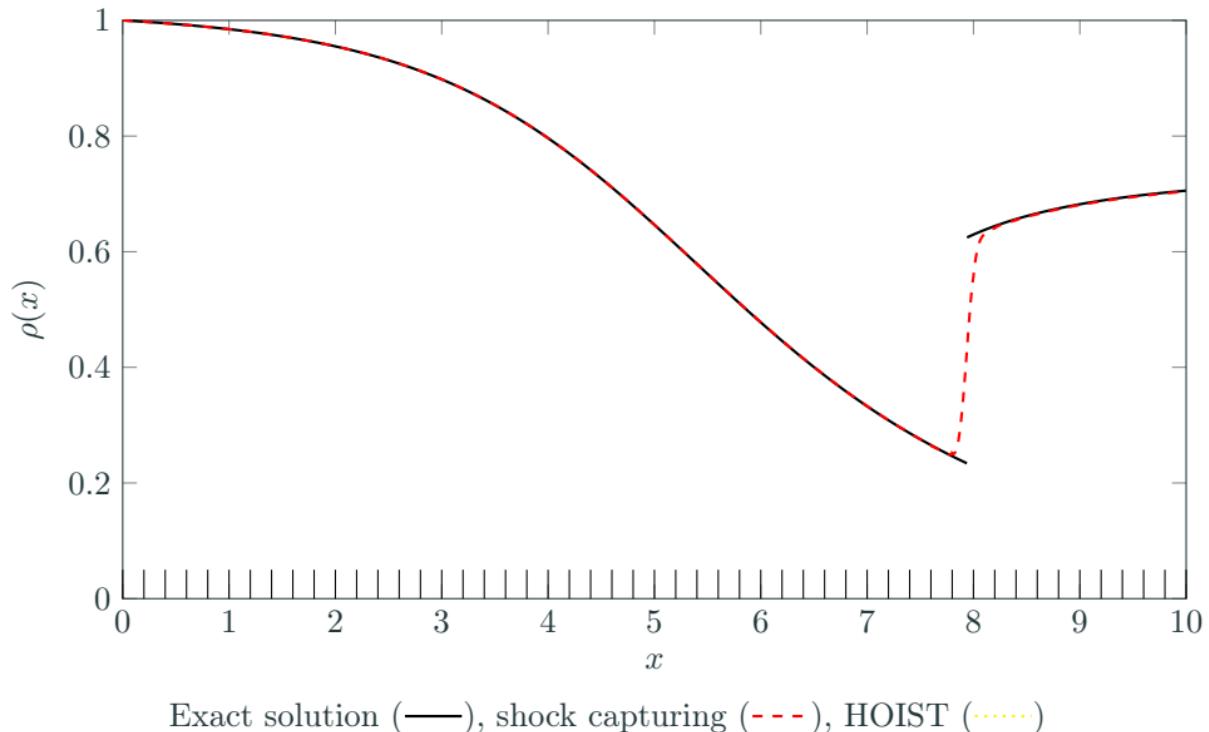


$p = 0$ space for solution, $q = 2$ space for mesh

Inviscid flow through area variation: HOIST vs capturing ($p = 4$)

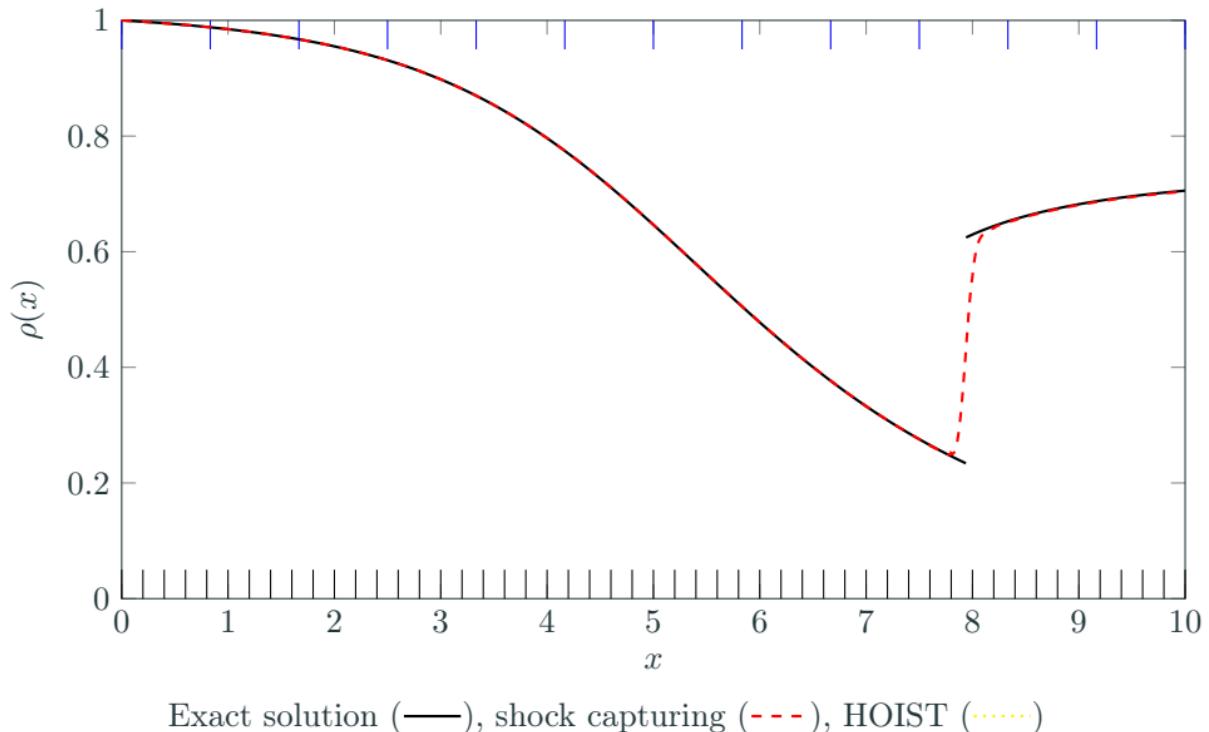


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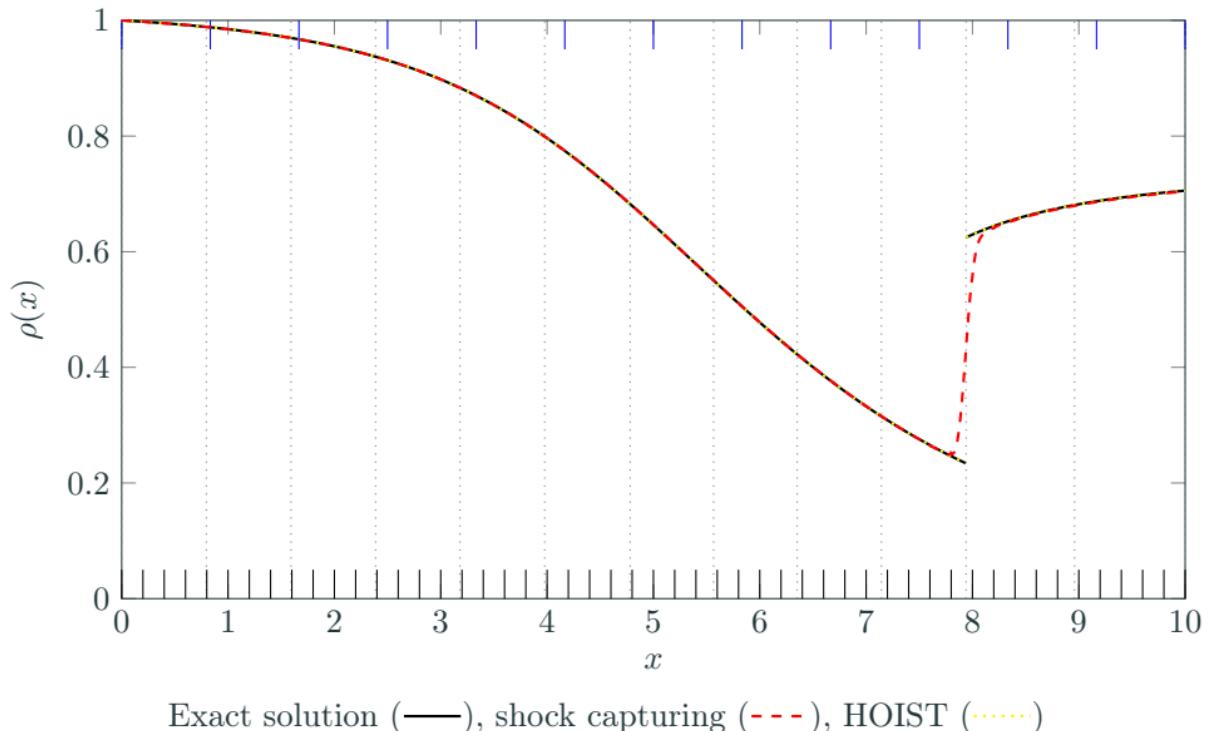
Exact solution (—), shock capturing (- - -), HOIST (.....)

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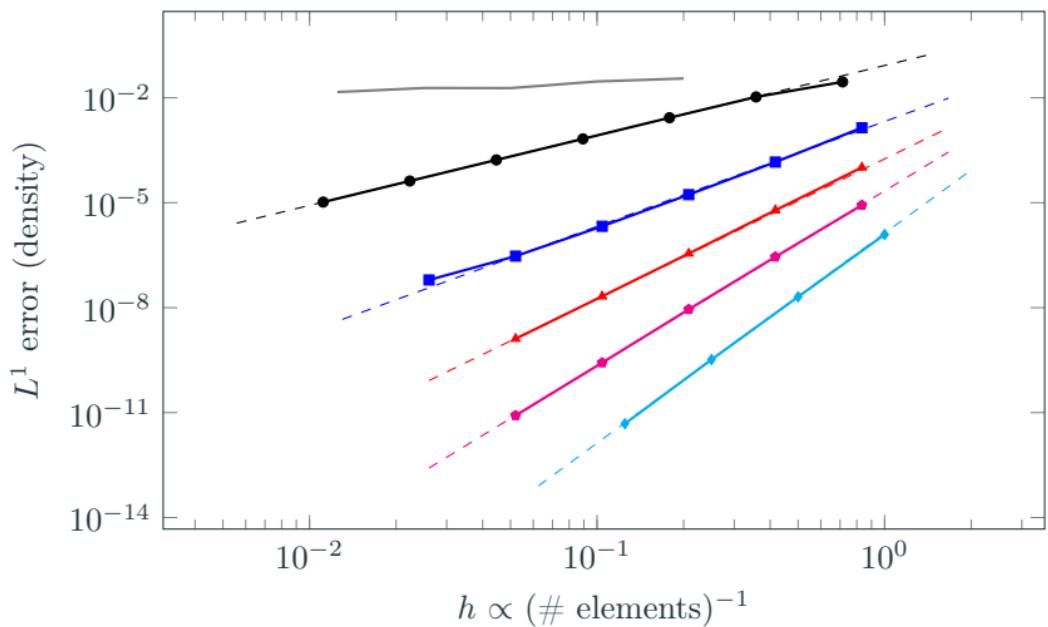


Exact solution (—), shock capturing (- - -), HOIST (.....)

Inviscid flow through area variation: HOIST vs capturing ($p = 4$)



Inviscid flow through area variation: h -convergence



Shock capturing: $p = 4$ (—); HOIST: $p = 1$ (●), $p = 2$ (■), $p = 3$ (→), $p = 4$ (●), $p = 5$ (←); dashed line indicates optimal convergence rate ($\mathcal{O}(h^{p+1})$)

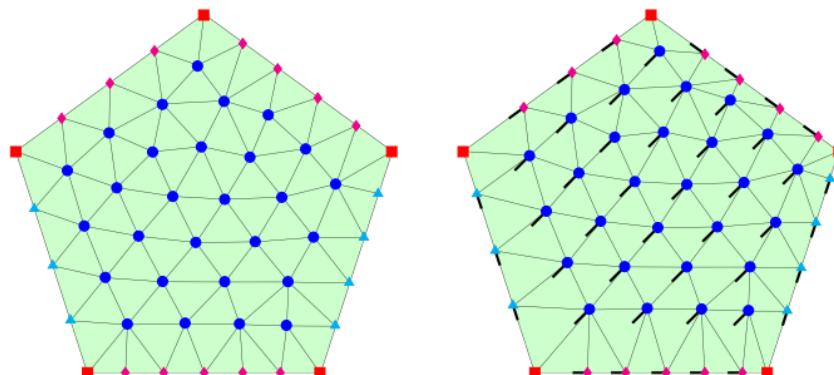
Observation: Shock capturing limited to first-order convergence rate; HOIST achieves optimal convergence rates ($\mathcal{O}(h^{p+1})$) and high accuracy per DoF

Construction of admissible mesh motion

Cannot directly optimize nodal coordinates (\mathbf{x}) without changing the domain; instead, construct mapping that guarantees mesh conforms to the domain boundaries from a collection of unconstrained degrees of freedom (\mathbf{y}) and directly optimize \mathbf{y}

$$\mathbf{x} = \phi(\mathbf{y}) \quad \Rightarrow \quad \begin{array}{ll} \text{minimize}_{\mathbf{u}, \mathbf{y}} & f(\mathbf{u}, \phi(\mathbf{y})) \\ \text{subject to} & \mathbf{r}(\mathbf{u}, \phi(\mathbf{y})) = \mathbf{0} \end{array}$$

- Planar boundaries: ϕ automatically constructed from normals

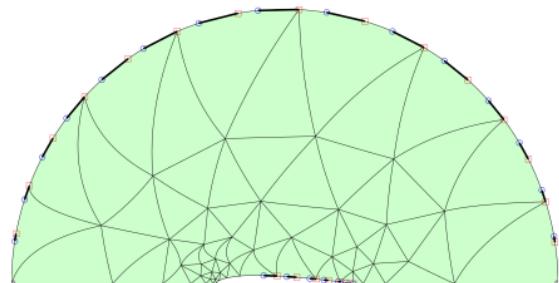
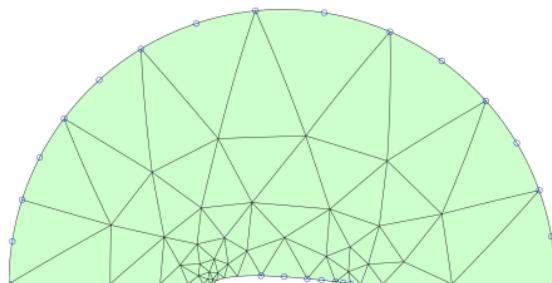


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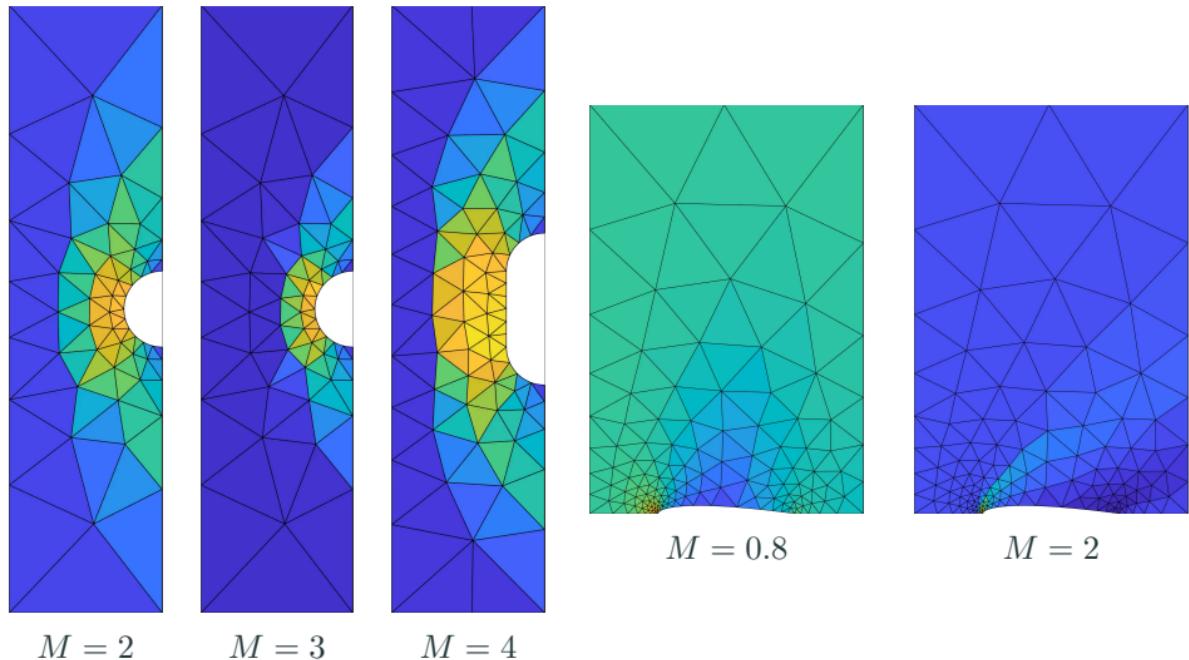
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- Planar boundaries: ϕ automatically constructed from normals
- Curved boundaries: ϕ defined from the analytical expression for the surface

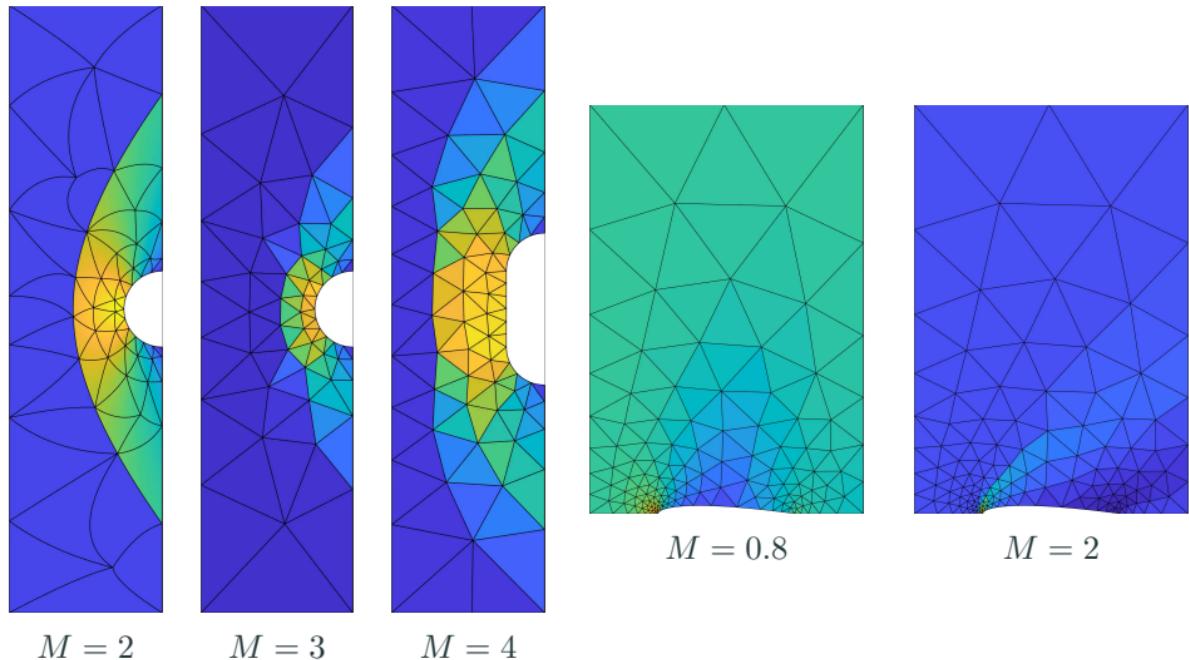


Implicit shock tracking for simple 2D compressible flows



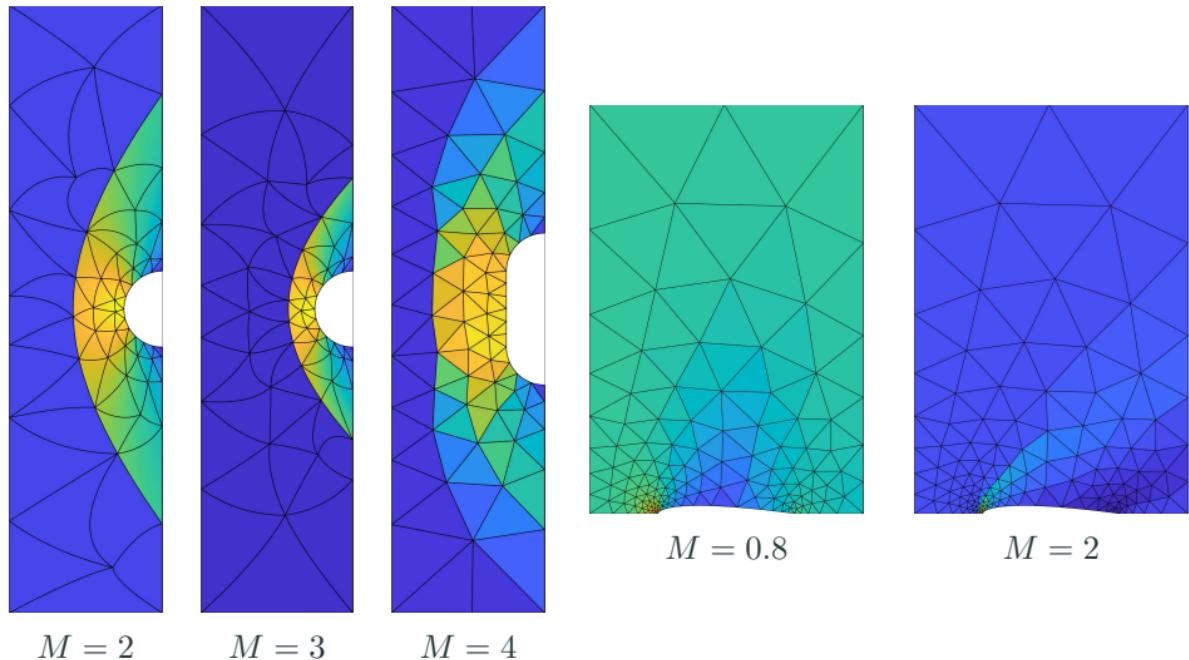
Observation: Quickly tracks bow shocks, shocks attached to curved boundaries, and secondary shocks; high-order elements curve to approximate curvature in shock surface; high-quality solutions on coarse high-order meshes ($\mathcal{O}(100)$ elements).

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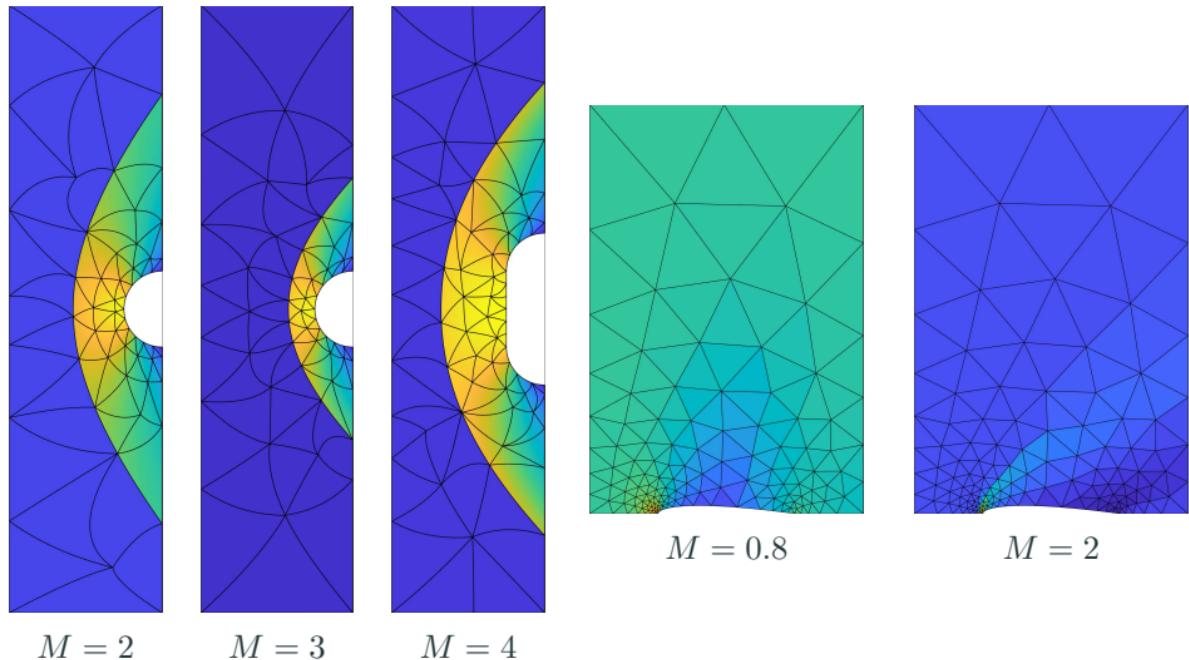
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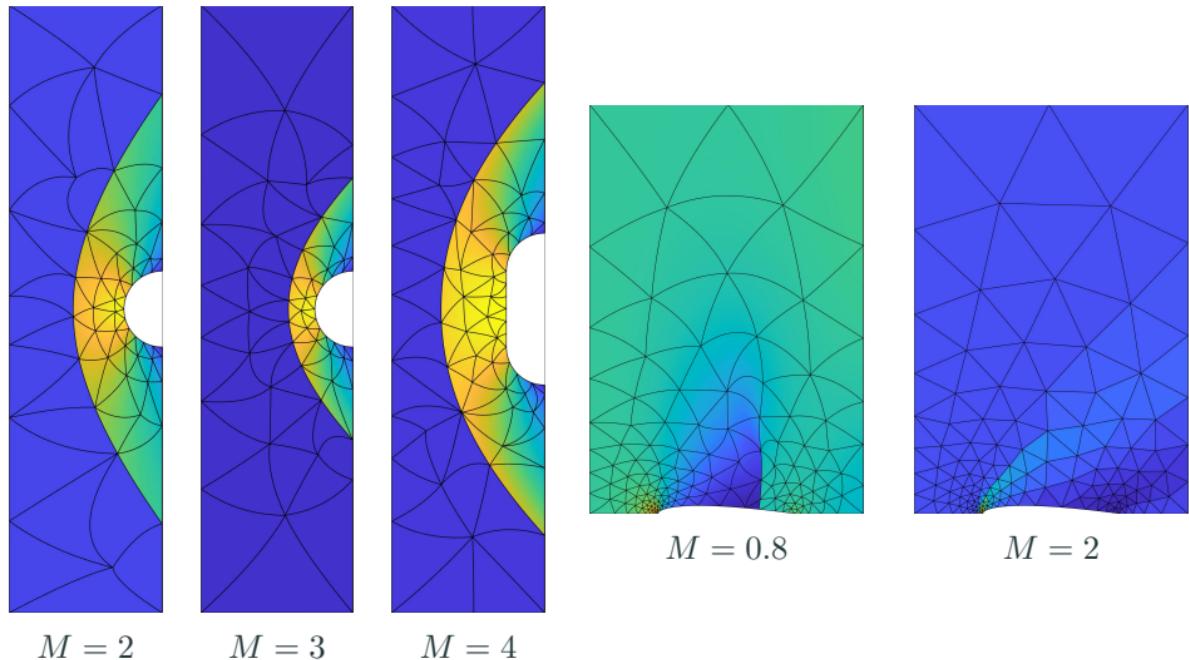
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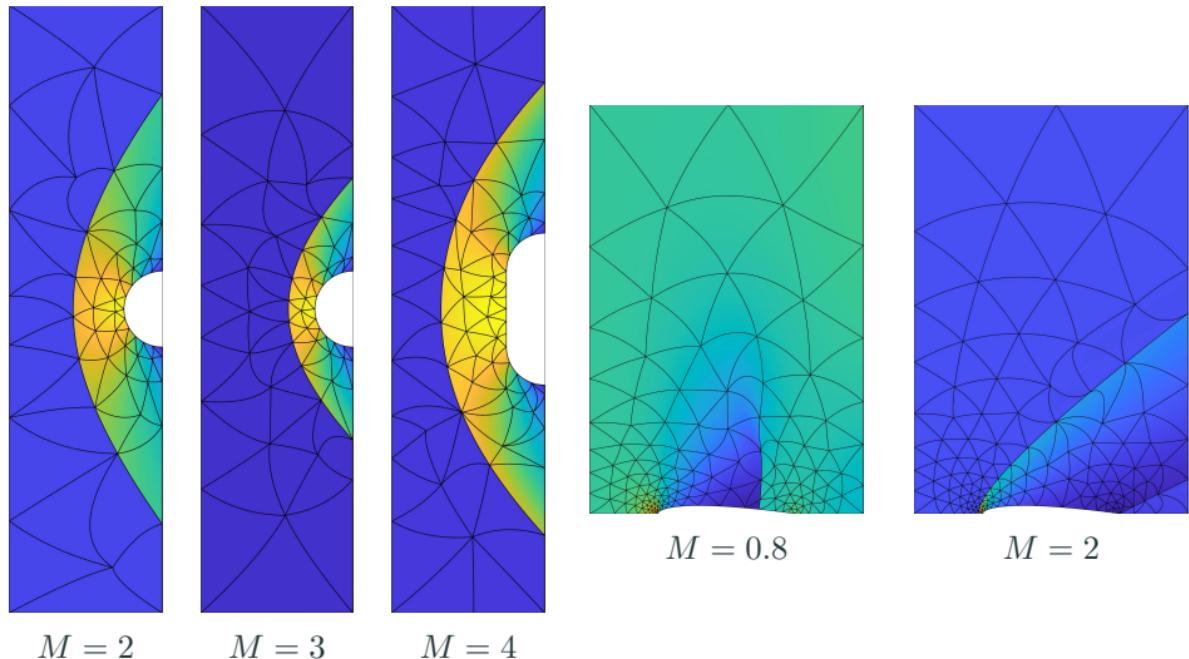
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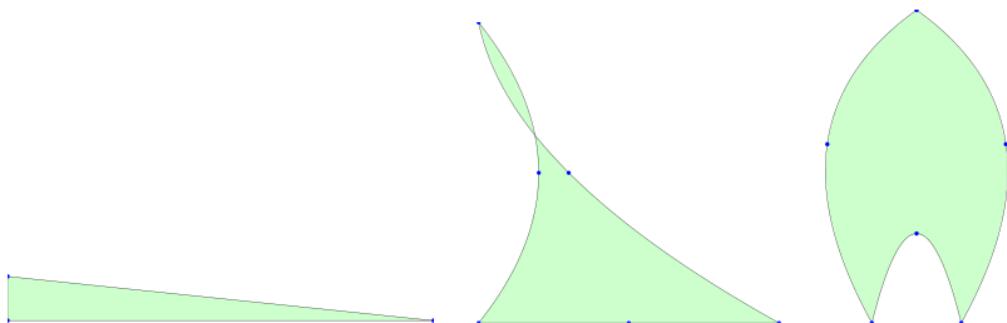


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Practical considerations: element collapse

Despite measures to keep mesh well-conditioned, best option can be to *remove* element from the mesh

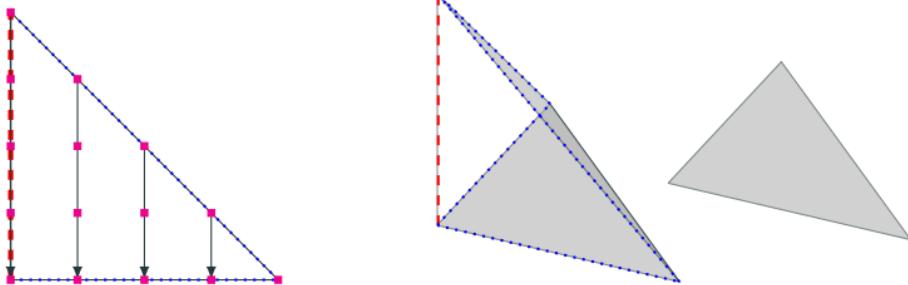
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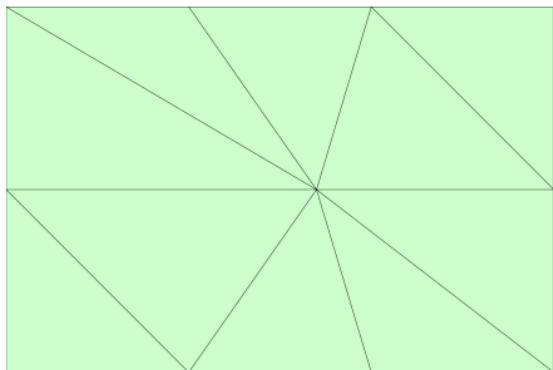
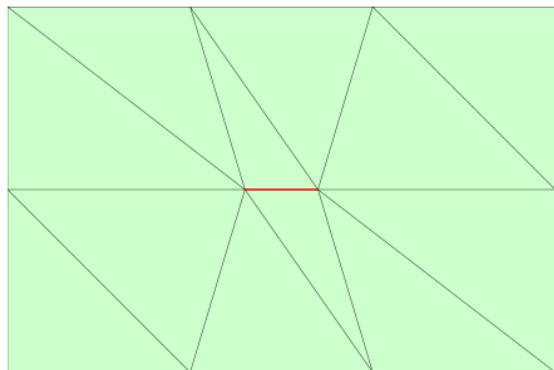
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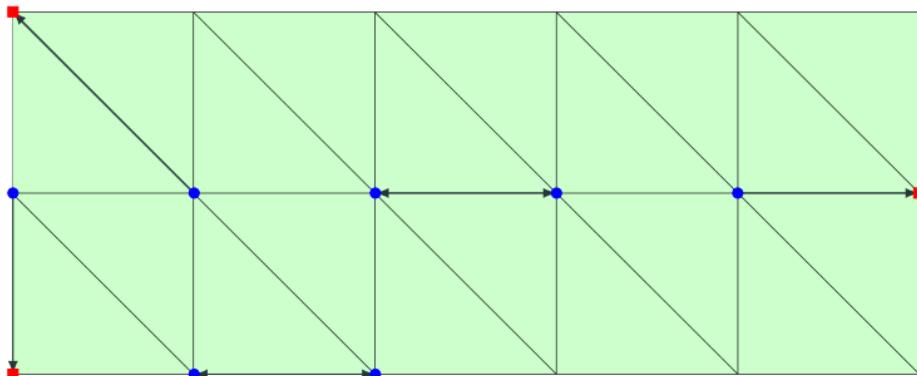
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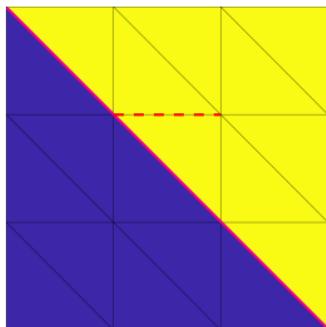
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- Remove all zero-volume elements
- Must preserve boundaries



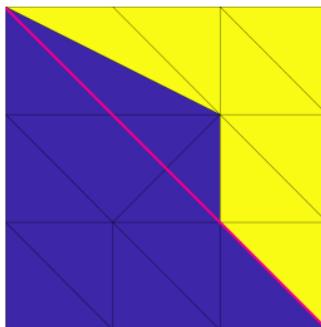
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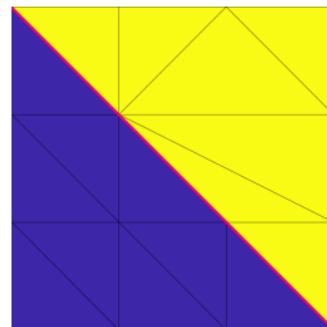
- Tag elements for removal based on volume, quality, edge length
- Collapse shortest edge: well-defined for simplices of any order in any dimension
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before collapse



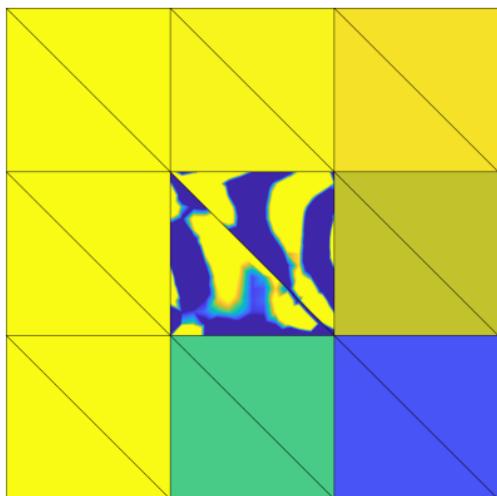
ignore shock



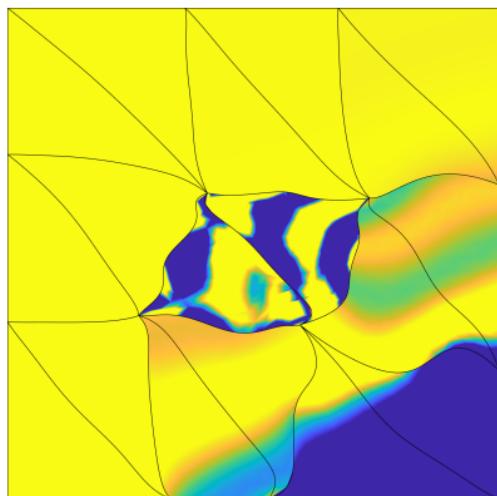
shock-aware

Practical considerations: solution re-initialization

- High-order solutions can become oscillatory, which leads to poor SQP steps (requiring many line search iterations)



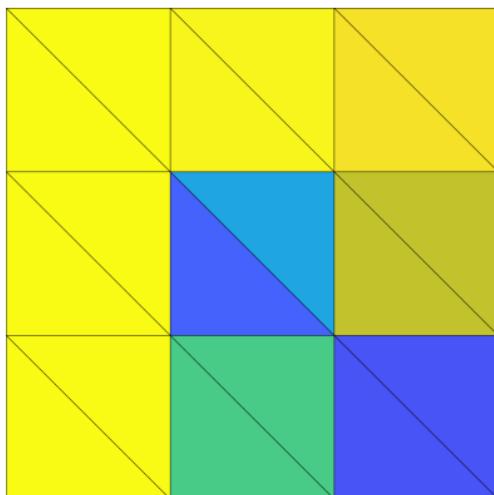
before SQP step (without re-init)



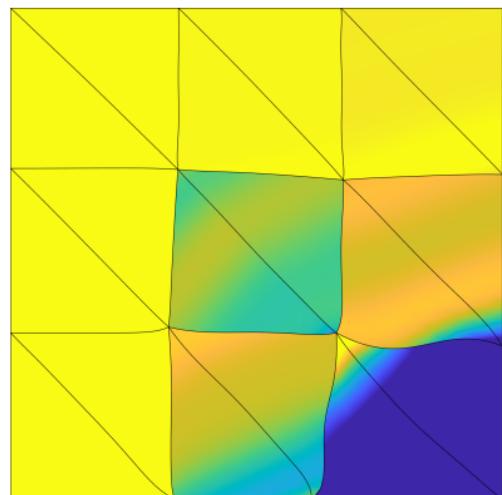
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- High-order solutions can become oscillatory, which leads to poor SQP steps (requiring many line search iterations)
- Overcome by replacing element-wise solution with the element-wise average (oscillatory element identified using Persson-Peraire indicator)



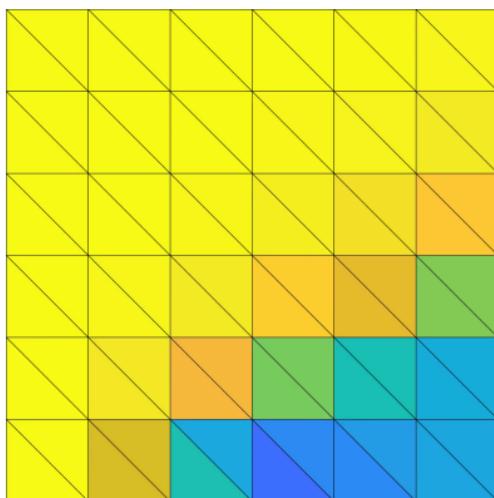
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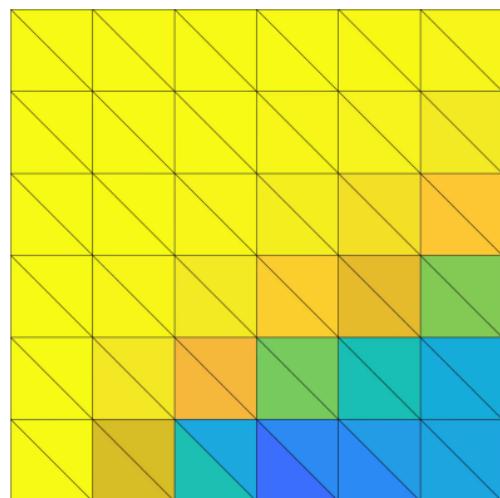
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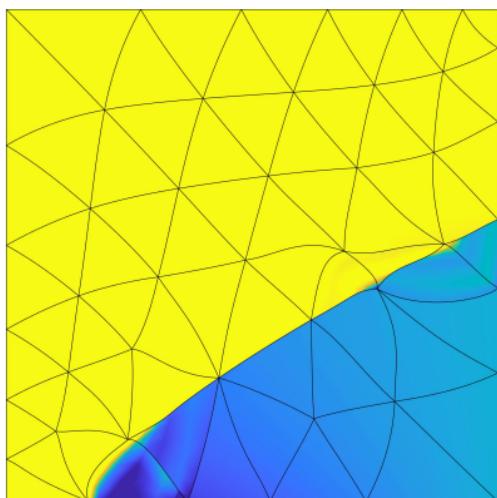
without re-initialization



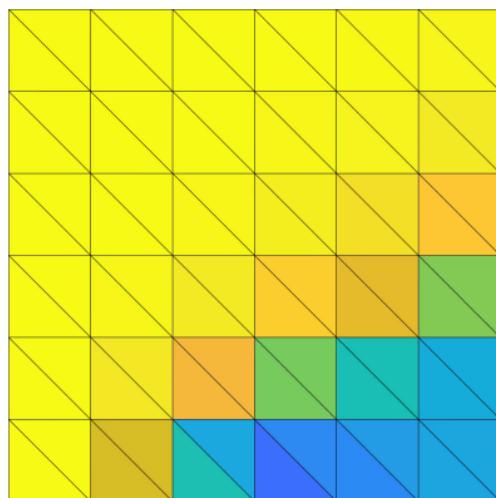
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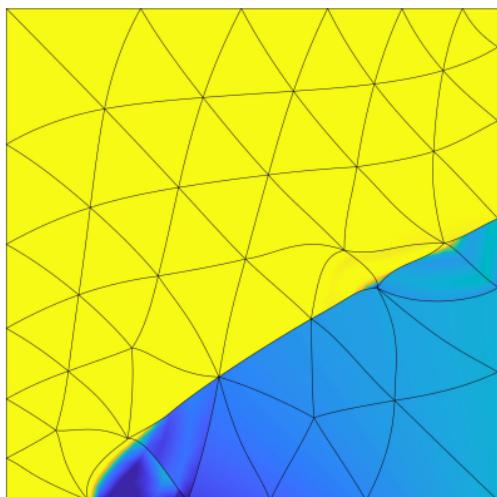
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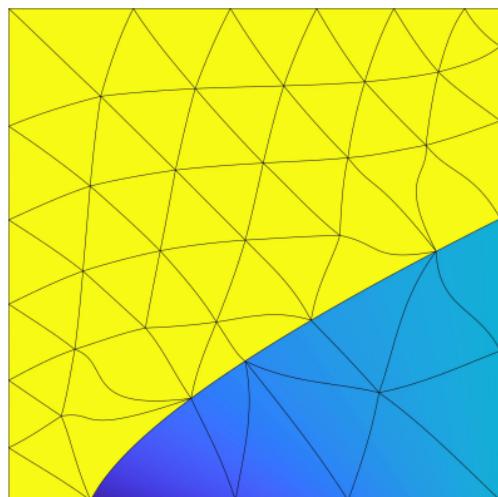
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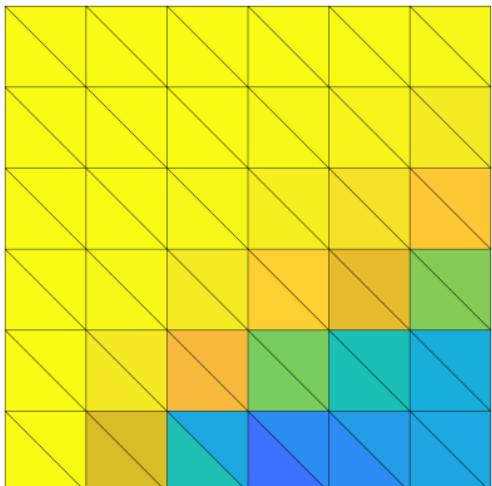
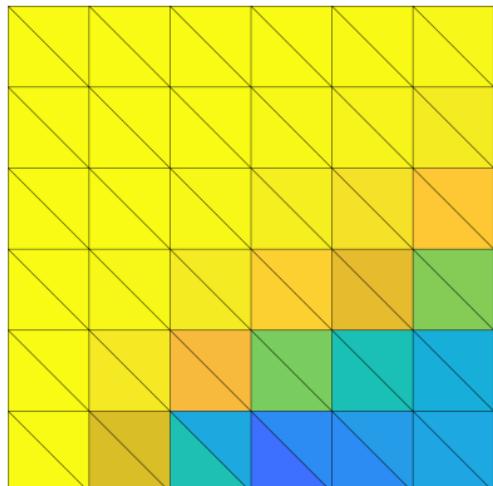


with re-initialization

Practical considerations: initialization

Robustness measures reduce sensitivity of solvers to initialization of \mathbf{u} , \mathbf{x} .

- \mathbf{x}_0 : directly from mesh generation
- \mathbf{u}_0 : DG($p = 0$) solution on mesh \mathbf{x}_0
- homotopy in p no longer required

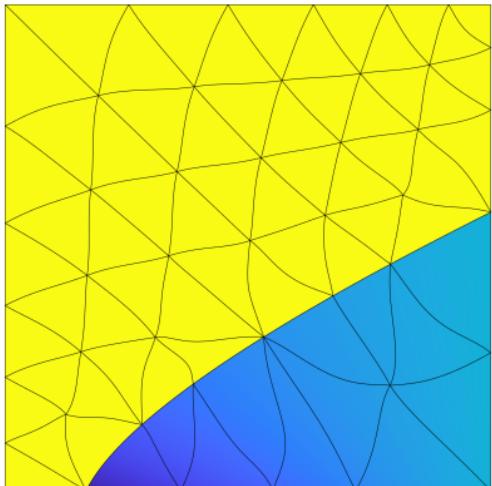
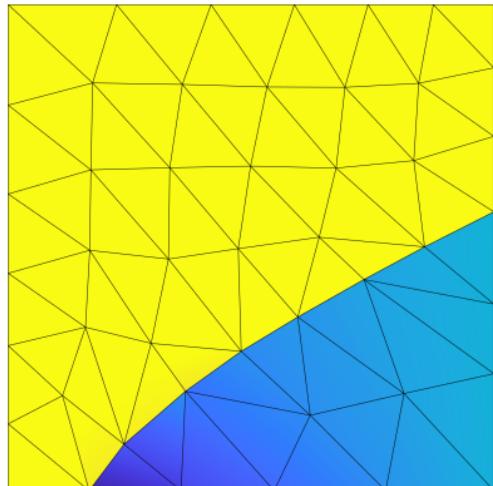


Reference mesh, $p = 0$ DG solution

Practical considerations: initialization

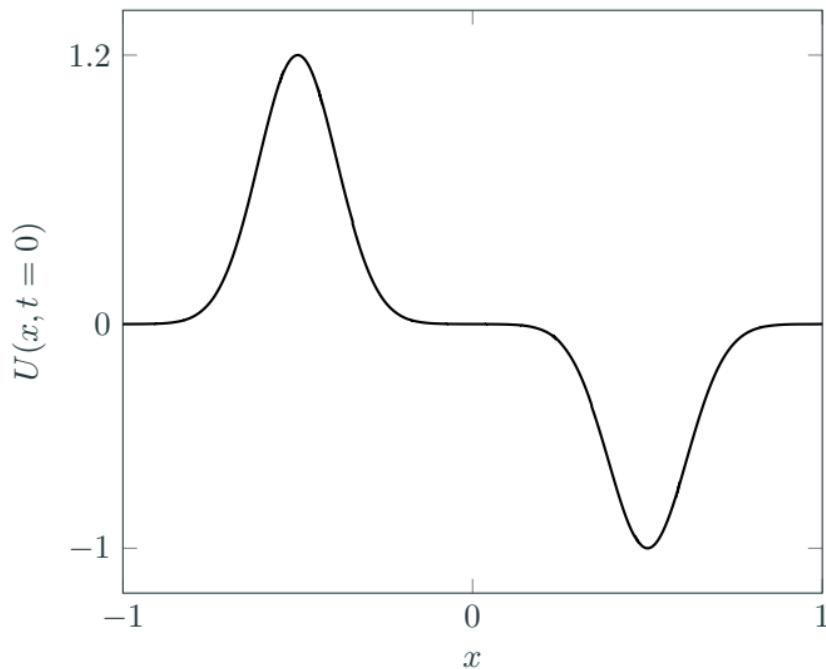
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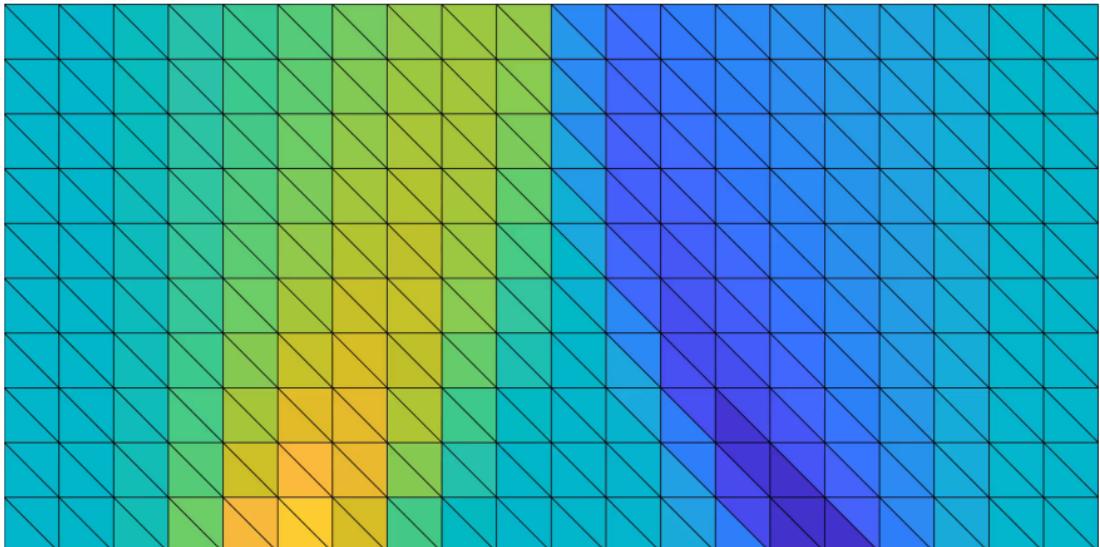


$p = 1$ (left) and $p = 4$ (right) tracking solution

Burgers' equation, shock formation and intersection



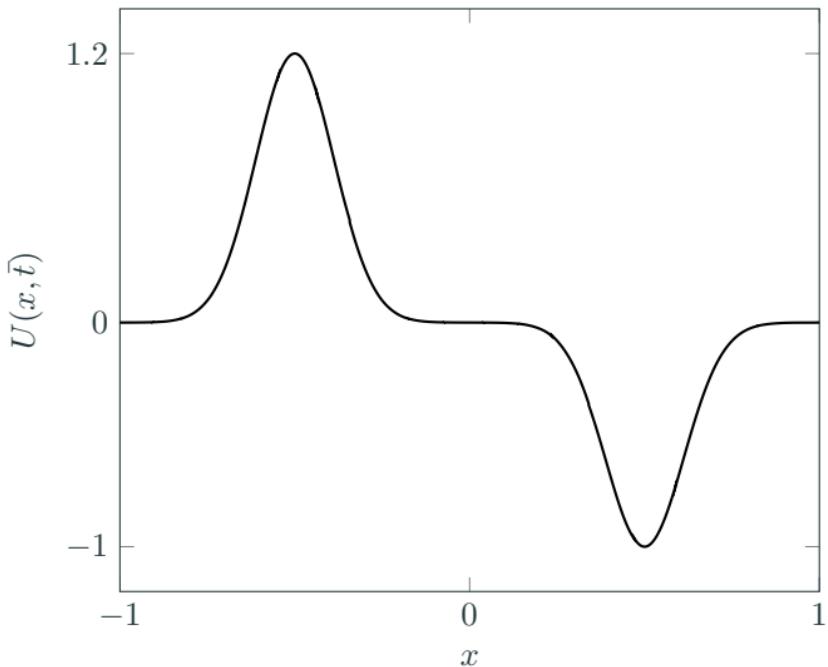
Burgers' equation, shock formation and intersection (space-time)



$$p = q = 3$$

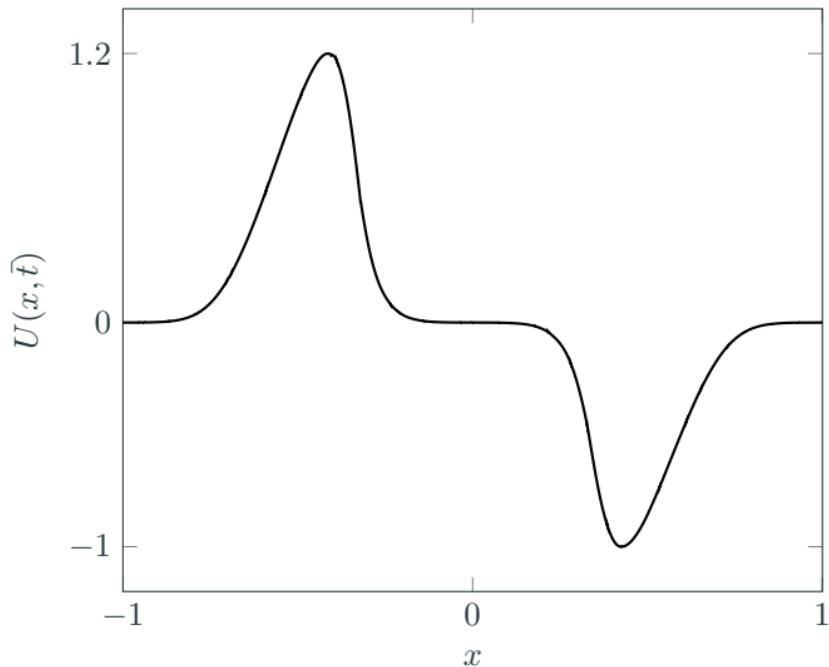
Observation: Triple point where shocks merge is tracked. Insufficient resolution to fully capture shock formation; approximate with discontinuity.

Burgers' equation, shock formation and intersection (time slices)



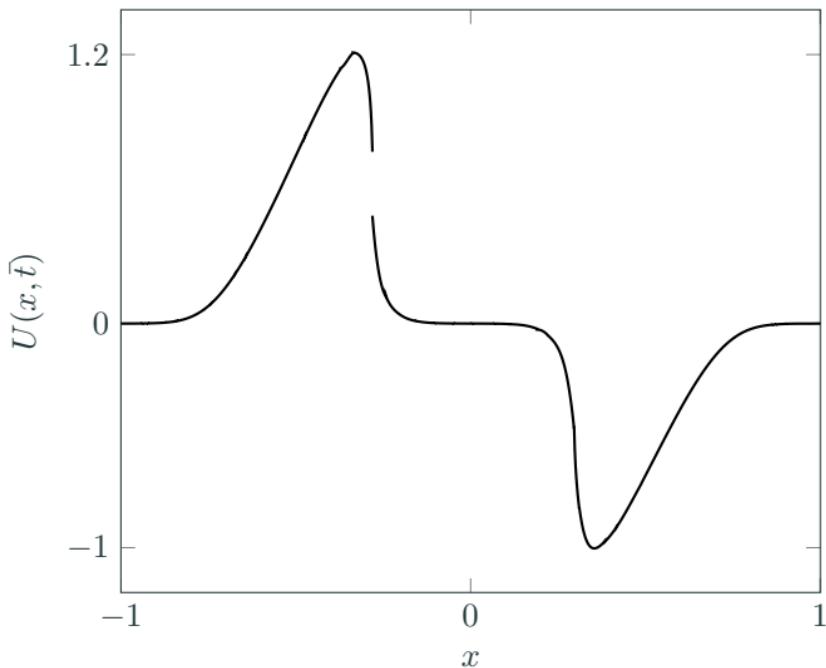
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Burgers' equation, shock formation and intersection (time slices)



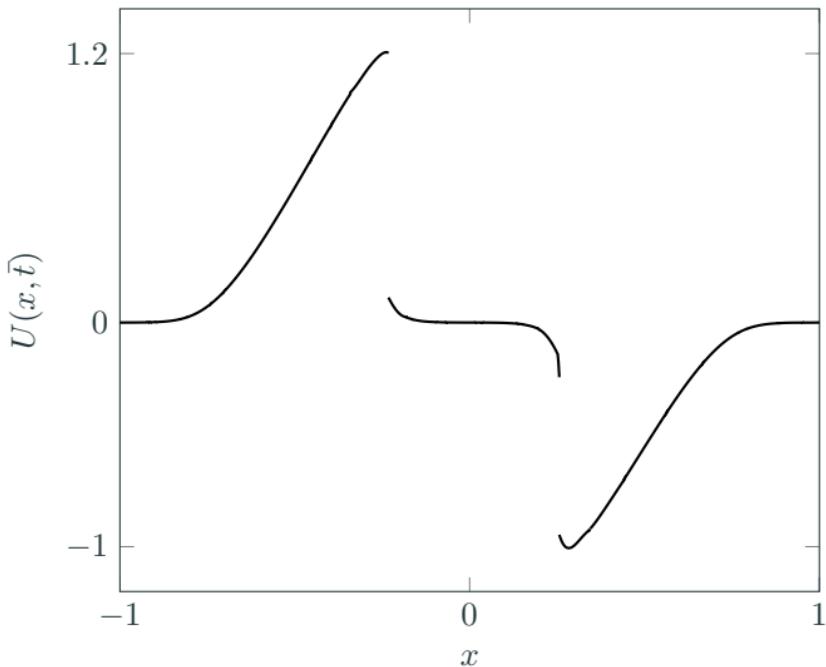
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Burgers' equation, shock formation and intersection (time slices)



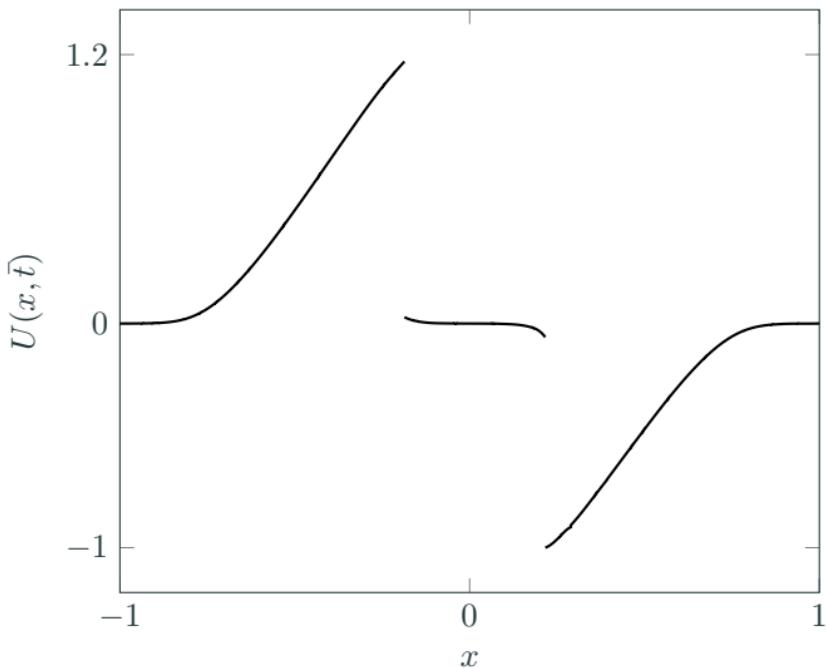
Observation: Triple point where shocks merge is tracked. Insufficient resolution to fully capture shock formation; approximate with discontinuity.

Burgers' equation, shock formation and intersection (time slices)



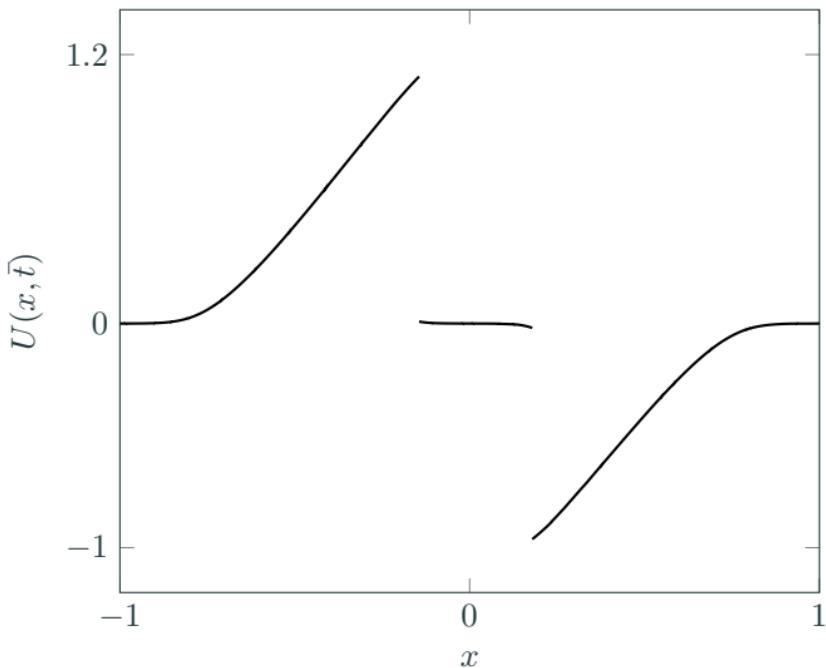
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Burgers' equation, shock formation and intersection (time slices)



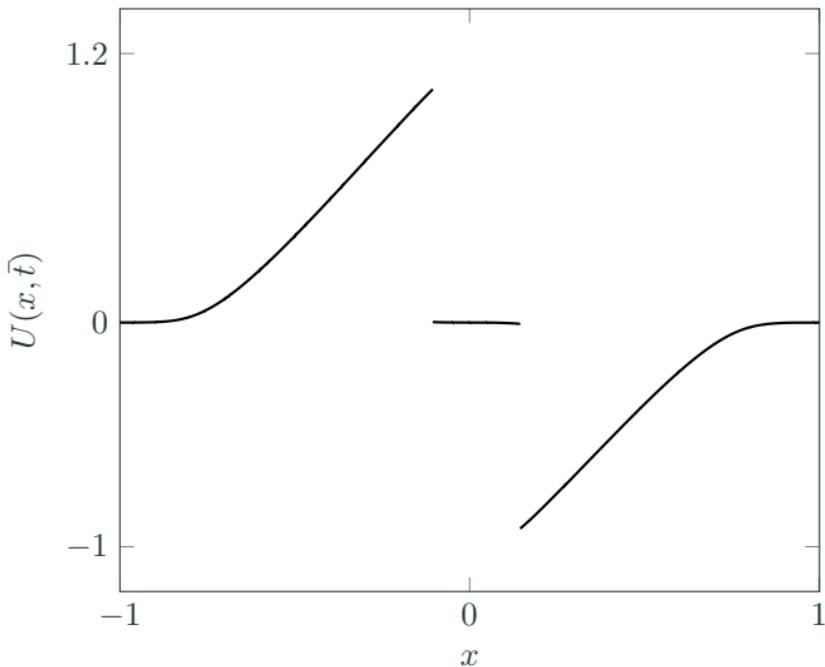
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Burgers' equation, shock formation and intersection (time slices)



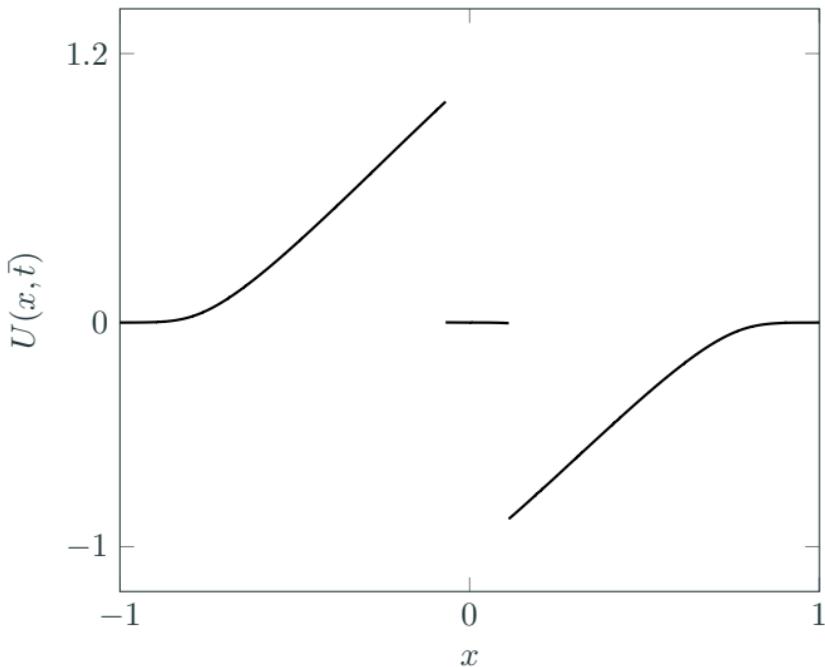
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Burgers' equation, shock formation and intersection (time slices)



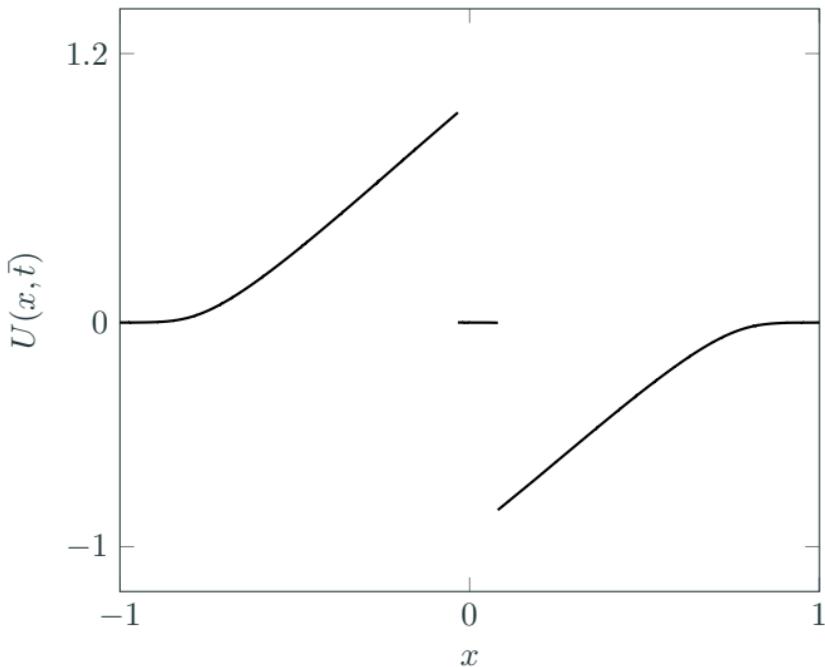
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Burgers' equation, shock formation and intersection (time slices)



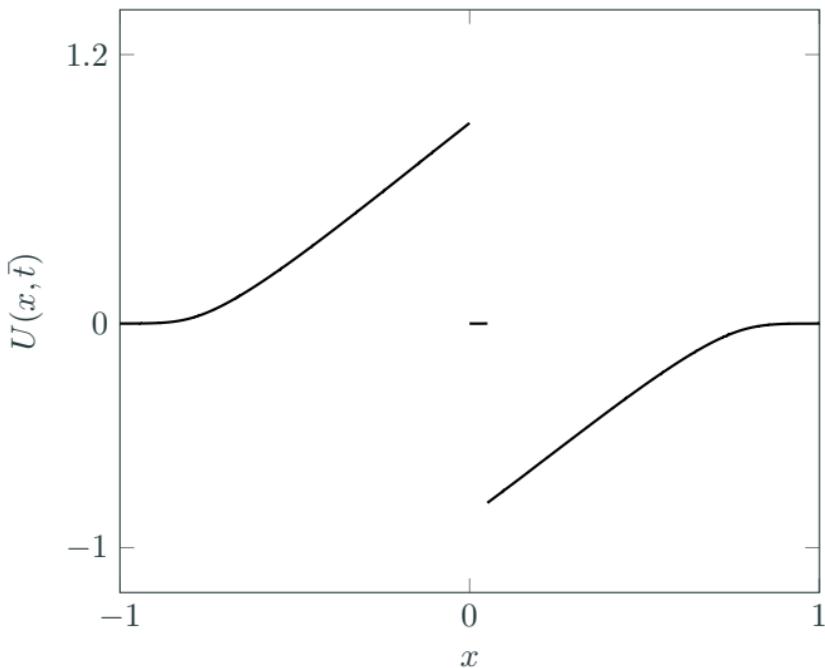
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Burgers' equation, shock formation and intersection (time slices)



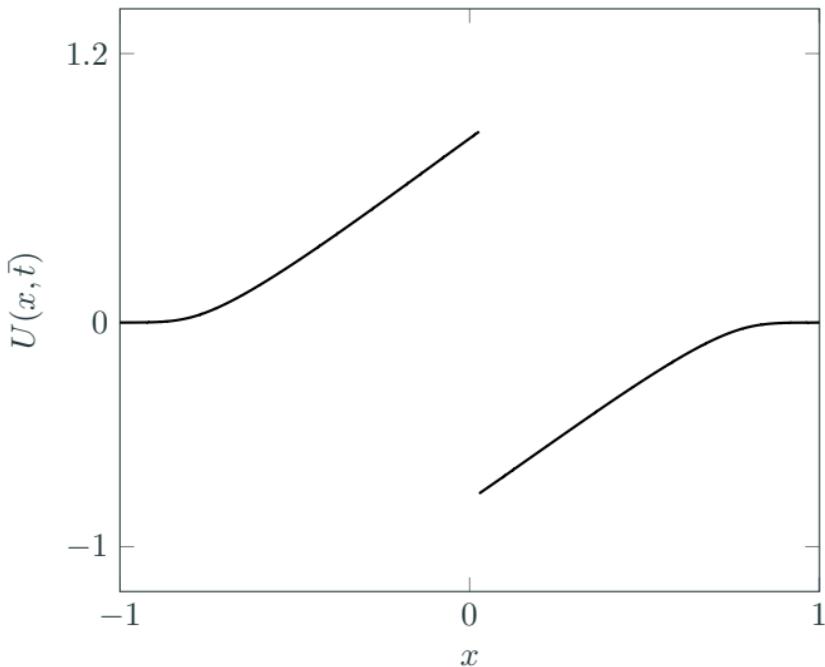
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Burgers' equation, shock formation and intersection (time slices)



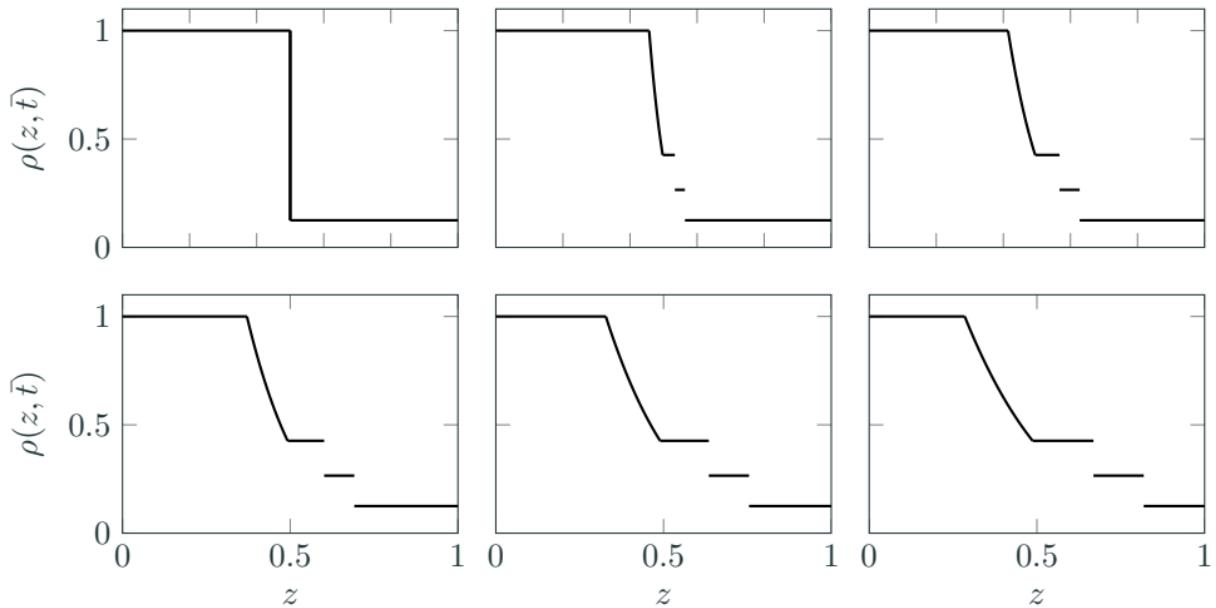
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Burgers' equation, shock formation and intersection (time slices)



Observation: Triple point where shocks merge is tracked. Insufficient resolution to fully capture shock formation; approximate with discontinuity.

Unsteady, inviscid flow, space-time: Sod shock tube



Unsteady, inviscid flow, space-time: Sod shock tube



$$p = 2, q = 1$$

Observation: Tracks multiple features including discontinuities and derivative jumps; stronger features “easier” to track (track earlier in process).

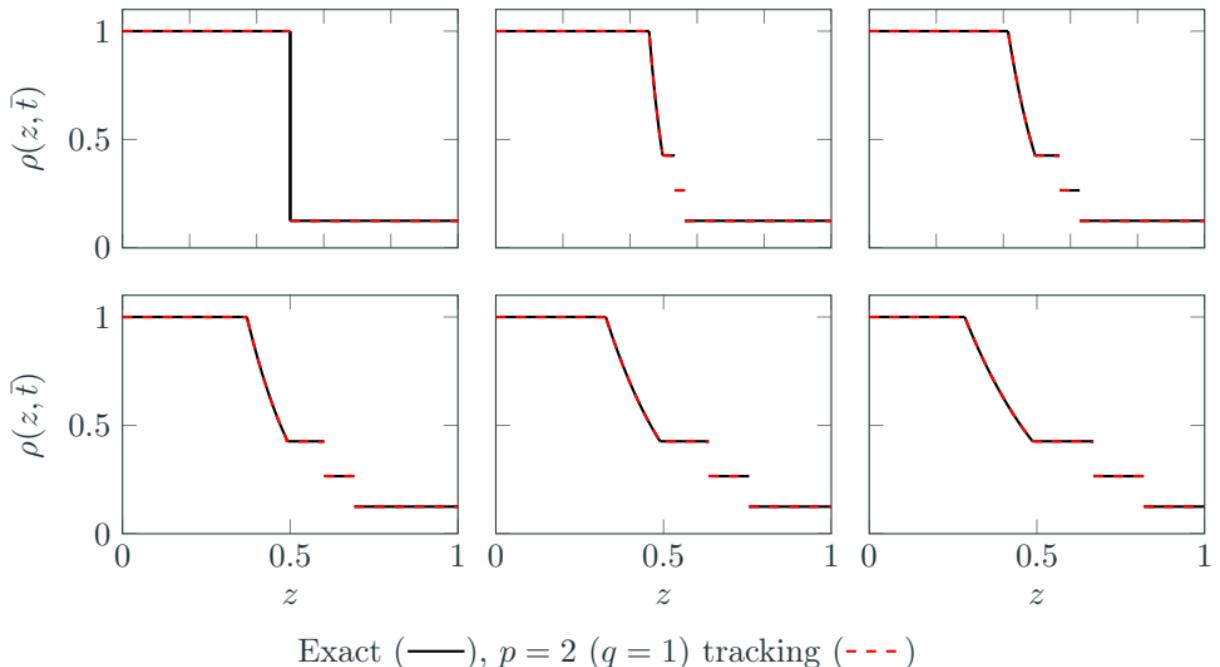
Unsteady, inviscid flow, space-time: Sod shock tube



$$p = 2, q = 1$$

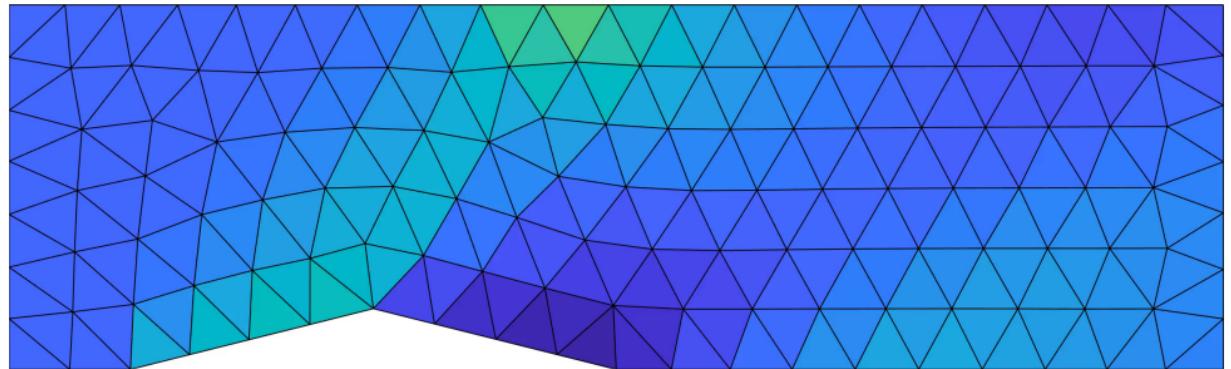
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Unsteady, inviscid flow, space-time: Sod shock tube



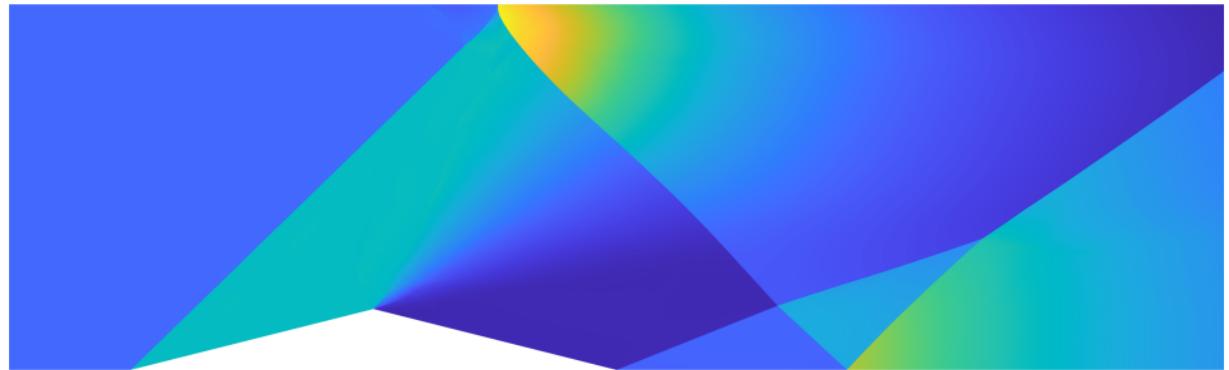
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2D Supersonic flow: $M = 2$ flow over diamond



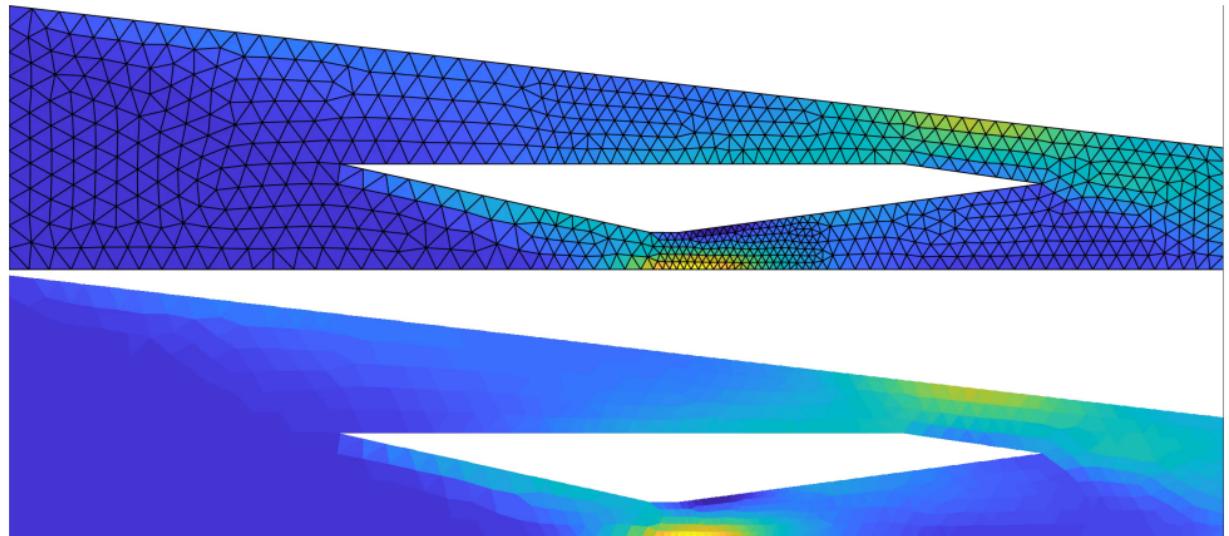
$$p = q = 2$$

2D Supersonic flow: $M = 2$ flow over diamond



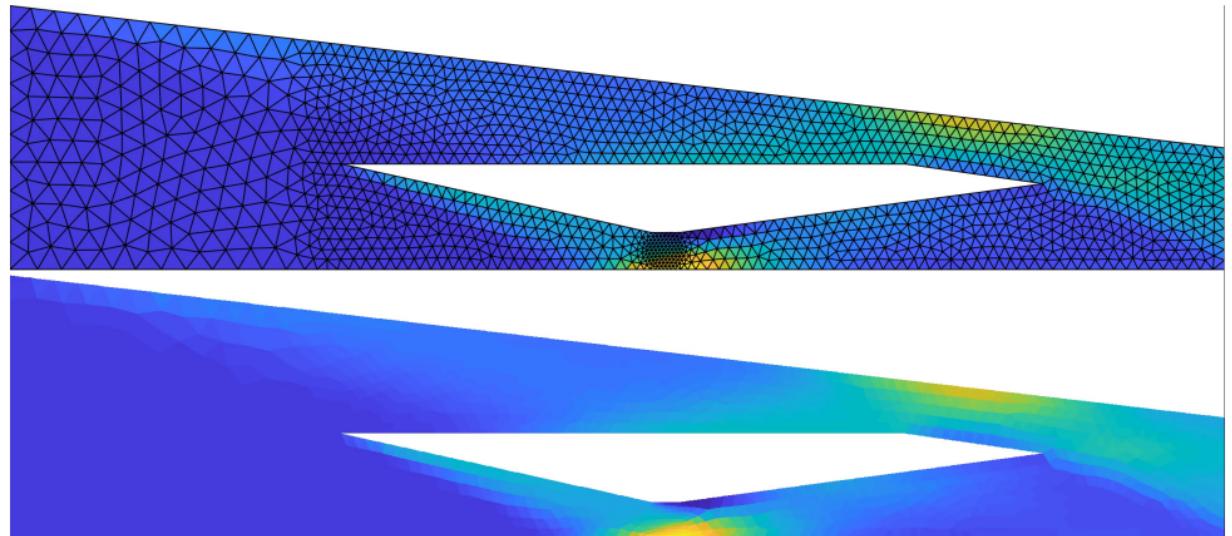
$$p = q = 2$$

2D Hypersonic flow: $M = 5$ flow through scramjet



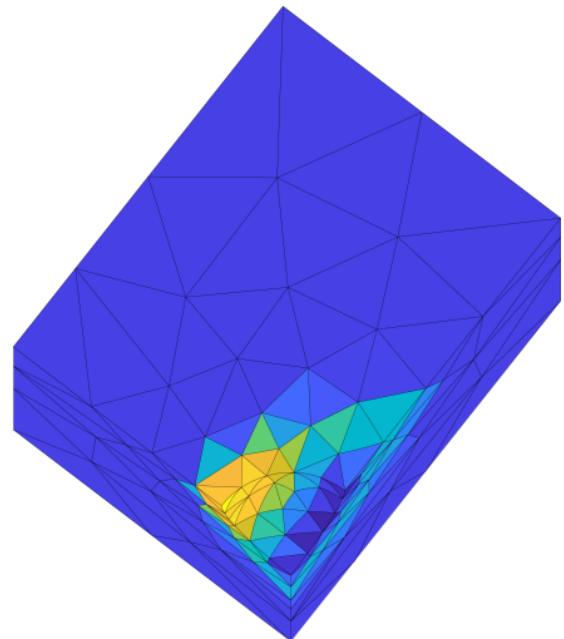
Coarse mesh, $p = q = 2$

2D Hypersonic flow: $M = 5$ flow through scramjet



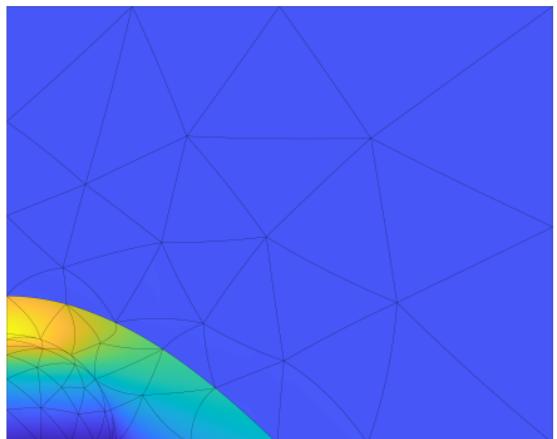
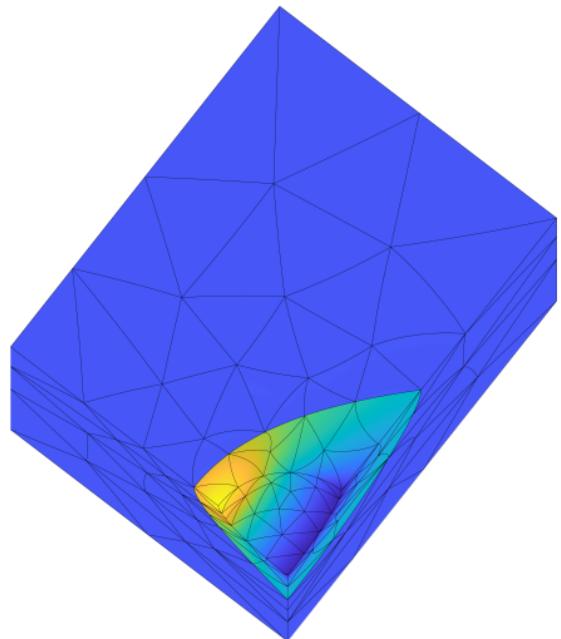
Fine mesh, $p = q = 2$

3D Supersonic flow: $M = 2$ flow over sphere



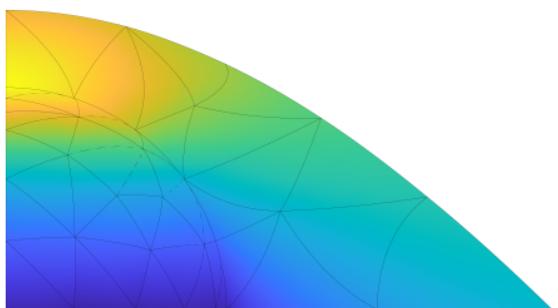
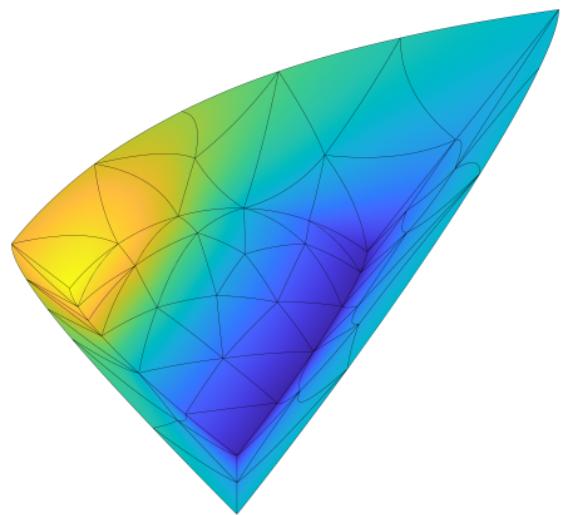
$$p = q = 2$$

3D Supersonic flow: $M = 2$ flow over sphere



$$p = q = 2$$

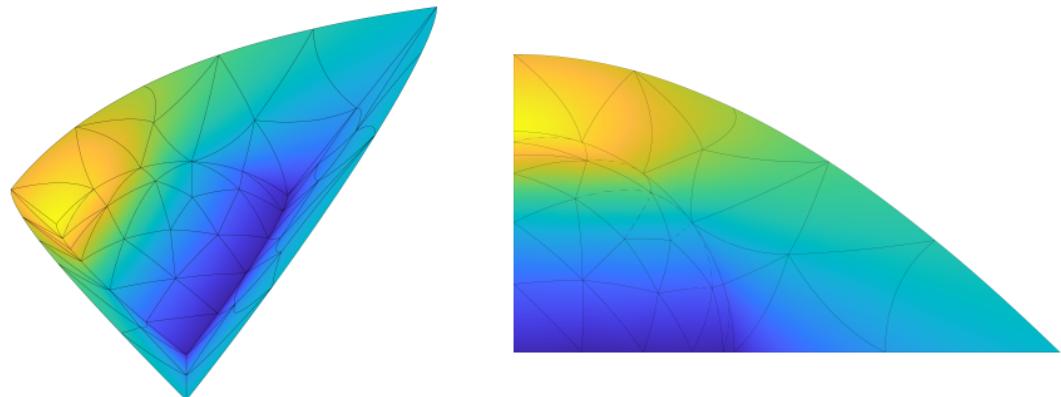
3D Supersonic flow: $M = 2$ flow over sphere



$$p = q = 2$$

High-order, implicit shock tracking

- **Implicit tracking:** formulate tracking as optimization problem over (\mathbf{u}, \mathbf{x})
- Highly *accurate solutions* on coarse meshes, *optimal convergence* rates
- High-order methods exaggerate accuracy benefits of tracking discontinuities
- Traditional barrier to tracking (explicitly meshing unknown discontinuity surface) replaced with solving constrained optimization problem



Research to make implicit tracking competitive for hypersonics

- Viscous conservation laws

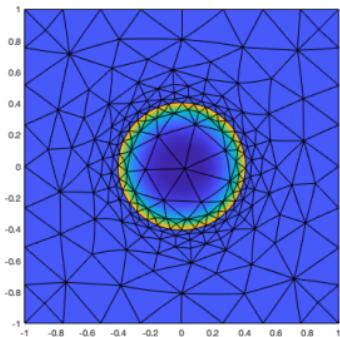
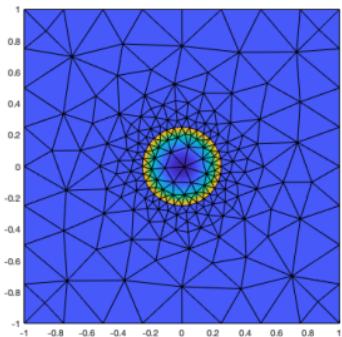
$$\begin{aligned} & \underset{\boldsymbol{u}, \boldsymbol{x}}{\text{minimize}} \quad \frac{1}{2} \|\boldsymbol{R}(\boldsymbol{u}, \boldsymbol{x})\|_2^2 + \frac{\kappa^2}{2} \|\boldsymbol{R}_{\text{msh}}(\boldsymbol{x})\|_2^2 \\ & \text{subject to} \quad \boldsymbol{r}(\boldsymbol{u}, \boldsymbol{x}) = \mathbf{0} \end{aligned}$$

Research to make implicit tracking competitive for hypersonics

- Viscous conservation laws
- Time-dependent problems:

Research to make implicit tracking competitive for hypersonics

- Viscous conservation laws
- Time-dependent problems: method of lines,



Research to make implicit tracking competitive for hypersonics

- Viscous conservation laws
- Time-dependent problems: method of lines, slab-based space-time



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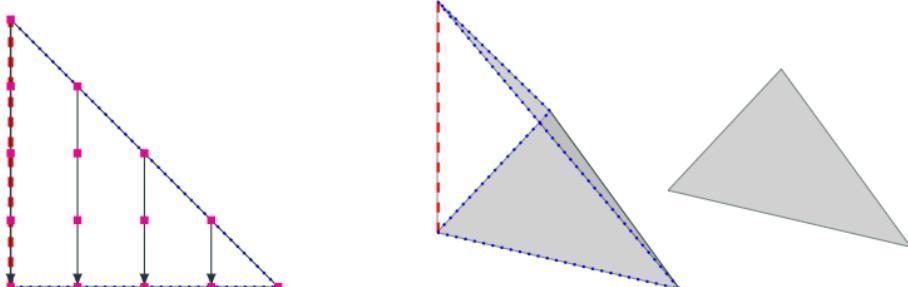
Research to make implicit tracking competitive for hypersonics

- Viscous conservation laws
- Time-dependent problems: method of lines, slab-based space-time
- Scalable linear system solver

$$\begin{bmatrix} B_{uu}(z_k, \hat{\lambda}(z_k)) & B_{ux}(z_k, \hat{\lambda}(z_k)) & J_u(z_k)^T \\ B_{ux}(z_k, \hat{\lambda}(z_k))^T & B_{xx}(z_k, \hat{\lambda}(z_k)) & J_x(z_k)^T \\ J_u(z_k) & J_x(z_k) & \mathbf{0} \end{bmatrix} \begin{bmatrix} \Delta u_k \\ \Delta x_k \\ \eta_k \end{bmatrix} = - \begin{bmatrix} g_u(z_k) \\ g_x(z_k) \\ r(z_k) \end{bmatrix}$$

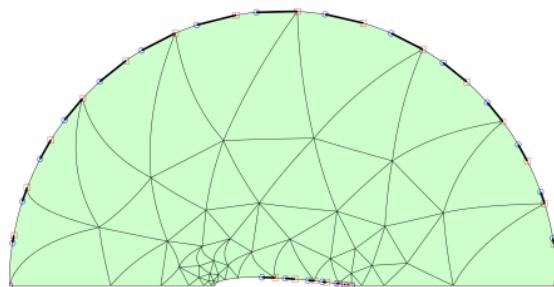
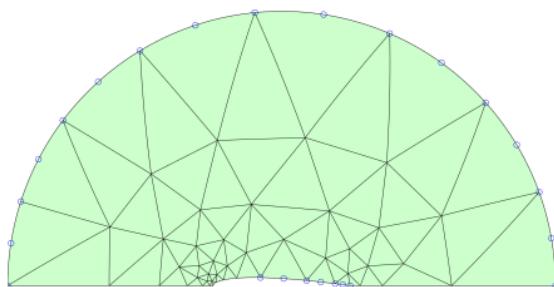
Research to make implicit tracking competitive for hypersonics

- Viscous conservation laws
- Time-dependent problems: method of lines, slab-based space-time
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- Edge collapses for hypercube elements; degenerate elements



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- Automatically slide nodes along curved boundaries from CAD or mesh



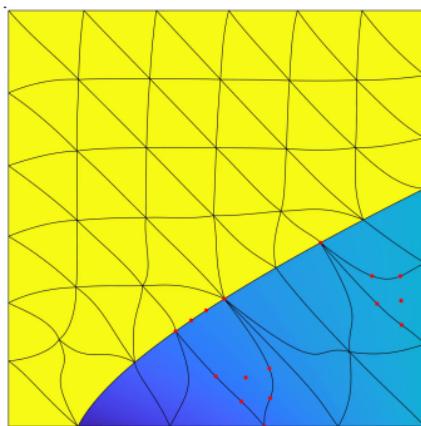
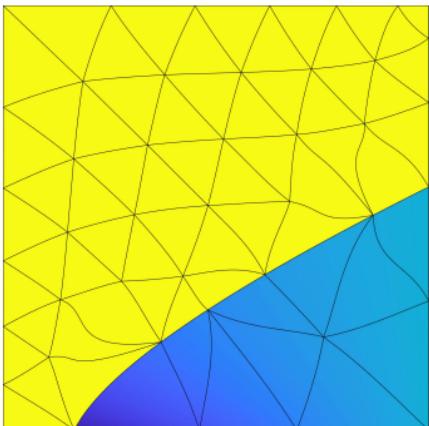
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- Integrate approach with second-order finite volume method
- Hybrid shock tracking/capturing approach (e.g., only track bow shock)



Perspective: artificial viscosity vs. implicit tracking

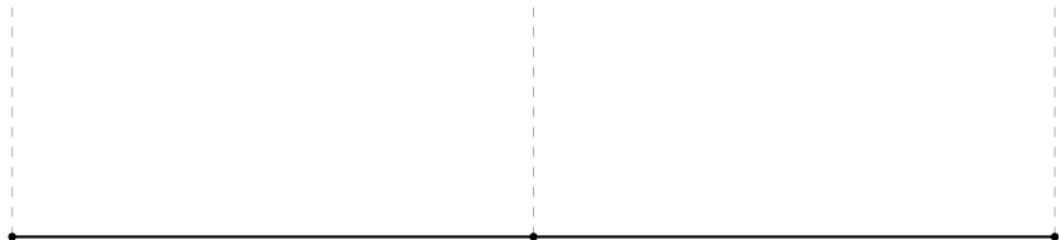
	artificial viscosity	implicit tracking ²
Strong shocks	control	easier
Complex shock structures	control	harder
Nonlinear solver	PTC/Newton	SQP
Parameter tweaking	formulation	solver
Linearization	∂_u, ∂_v	∂_u, ∂_x
Mesh generation	control	easier
Geometry	only high-order mesh	geometry required
Linear solver	ILU+GMRES	?
Cost per element	control	higher
Cost per iteration	control	higher
Mesh fineness	control	coarser
Overall cost	control	?

²e.g., HOIST, MDG-ICE

References i

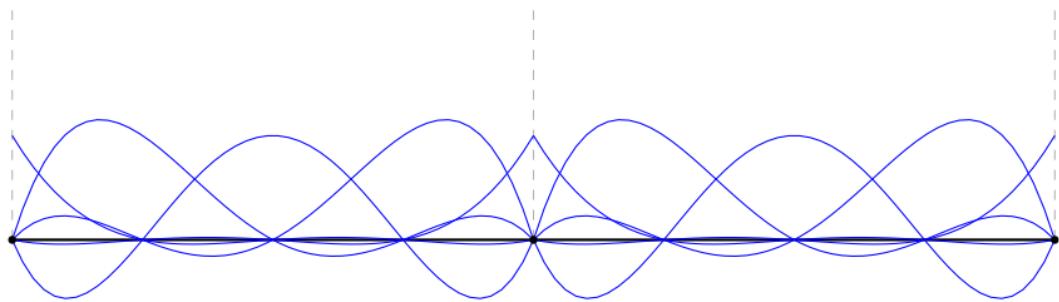
-  Corrigan, A., Kercher, A., and Kessler, D. (2019).
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International Journal for Numerical Methods in Fluids, 89(9):362–406.
-  Zahr, M. and Persson, P.-O. (2018).
An optimization-based approach for high-order accurate discretization of conservation laws with discontinuous solutions.
Journal of Computational Physics, 365:105–134.
-  Zahr, M., Shi, A., and Persson, P.-O. (2020).
Implicit shock tracking using an optimization-based discontinuous galerkin method.
Journal of Computational Physics.

Numerical methods for resolving shocks



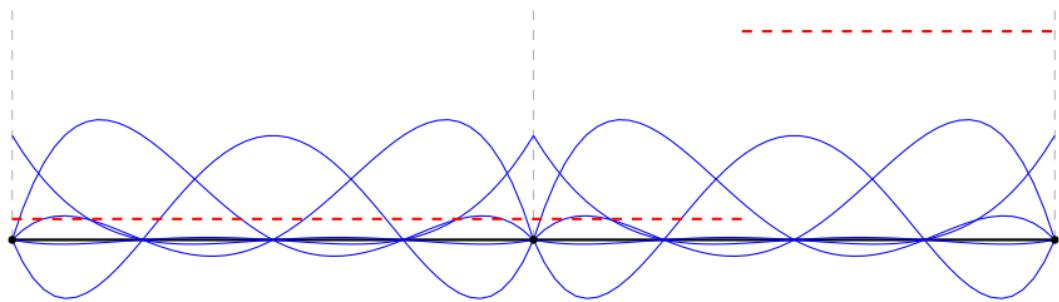
Fundamental issue: approximate discontinuity with polynomial basis

Numerical methods for resolving shocks



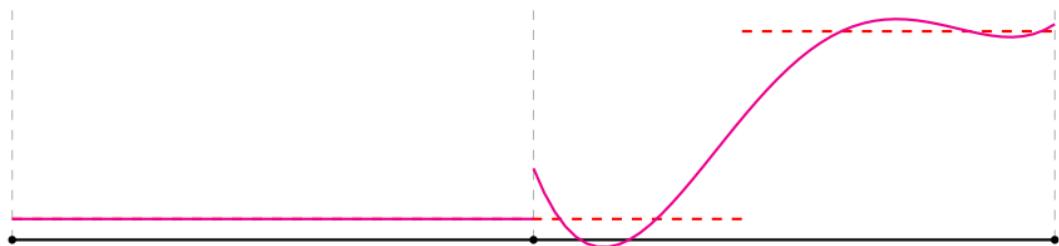
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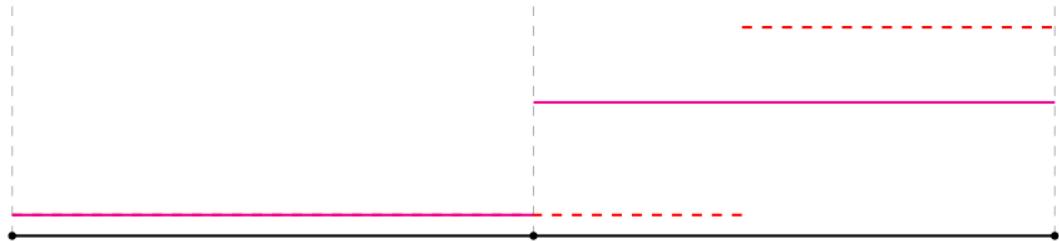
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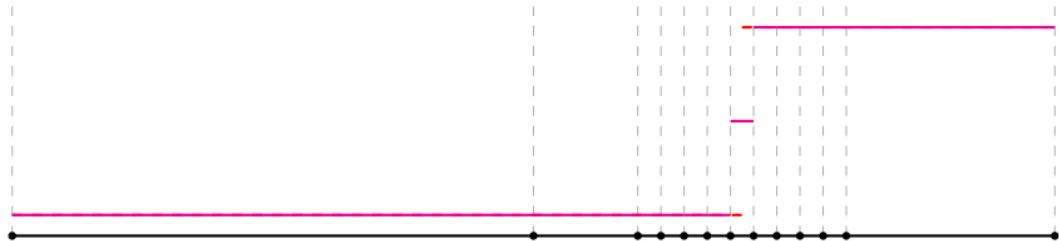


Fundamental issue: approximate discontinuity with polynomial basis

Existing solutions: **limiting**, artificial viscosity

Drawbacks: order reduction, local refinement

Numerical methods for resolving shocks

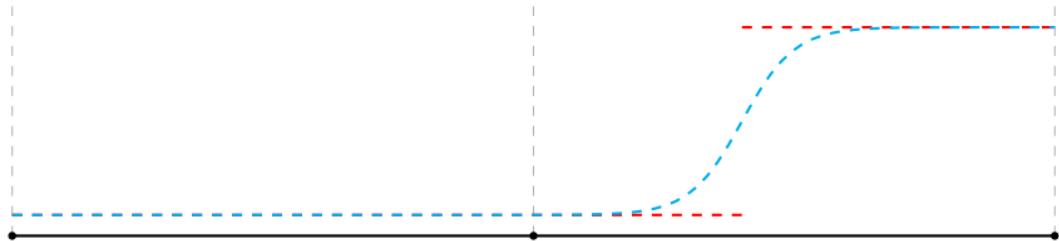


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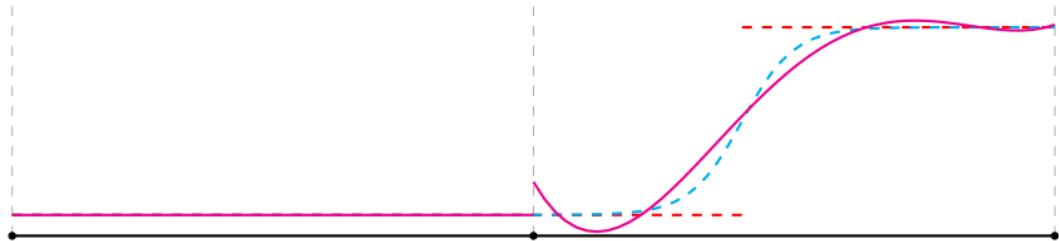


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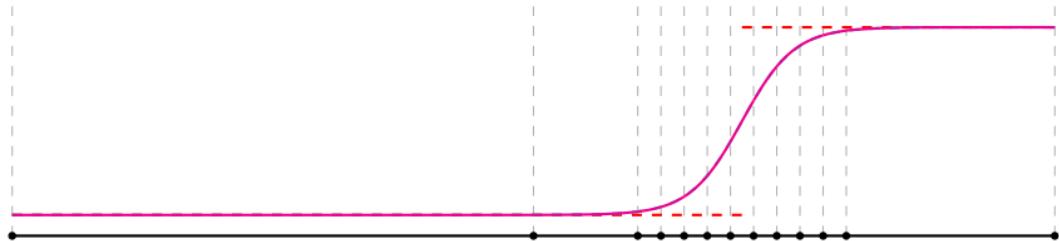


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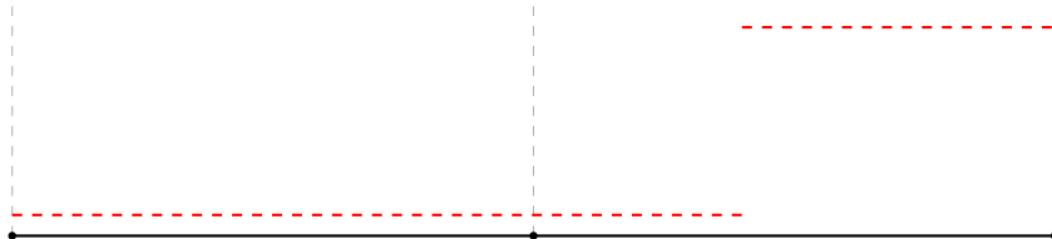


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Shock tracking/fitting: align features of solution basis with features in the solution using optimization formulation and solver

Numerical methods for resolving shocks



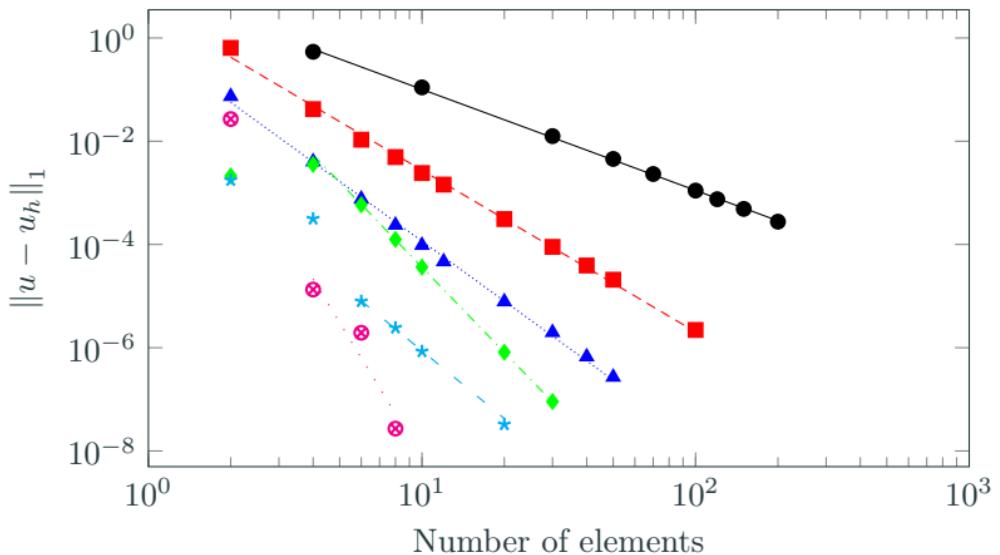
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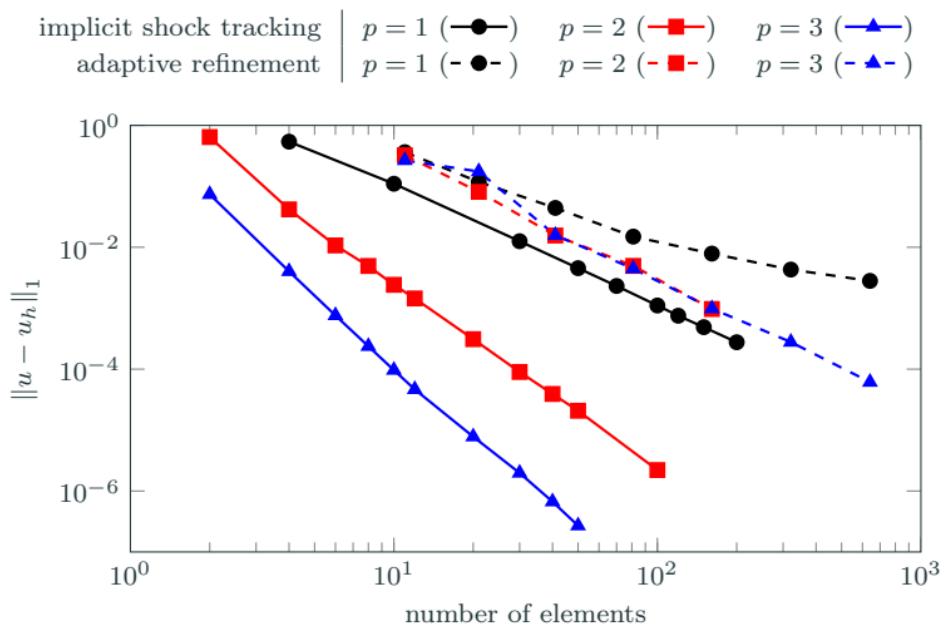
Why tracking: Recover optimal $\mathcal{O}(h^{p+1})$ convergence rates



Convergence of implicit shock tracking (Burgers' equation) with polynomial degrees $p = 1$ (\bullet),
 $p = 2$ (\blacksquare), $p = 3$ (\blacktriangle), $p = 4$ (\blacklozenge), $p = 5$ (\ast), $p = 6$ (\otimes).

Key observation: Optimal convergence rates ($\mathcal{O}(h^{p+1})$) attainable, even for discontinuous solutions.

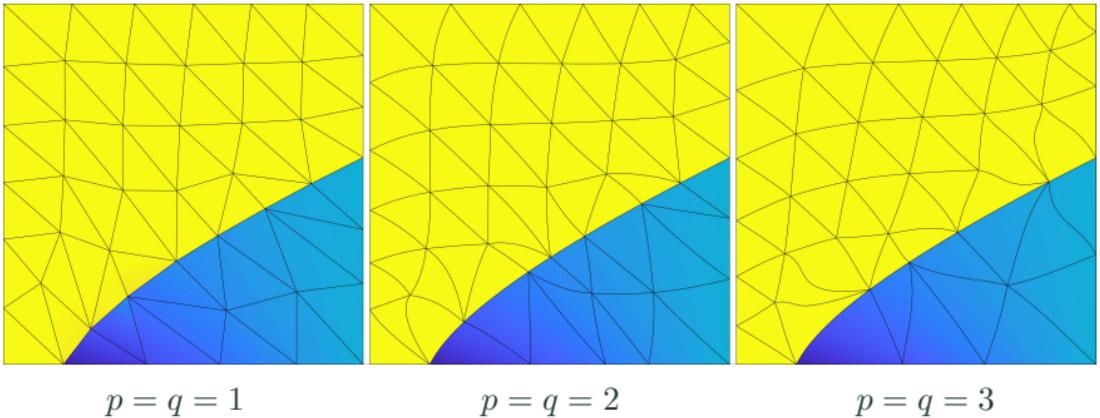
Why high-order tracking: Benefits more dramatic than low-order



Convergence of implicit shock tracking (Burgers' equation): implicit shock tracking (solid) vs. adaptive mesh refinement (dashed).

Key observation: Accuracy improvement of tracking approach relative to (specialized) adaptive mesh refinement is more exaggerated for high-order approximations: $\mathcal{O}(10^1)$ for $p = 1$ and $\mathcal{O}(10^6)$ for $p = 3$.

Burgers' equation, accelerating shock



Burgers' equation, accelerating shock: h convergence

Convergence of solution error (E_u) along line $x = 0.8$ and shock surface error (E_Γ)

p	q	$ \mathcal{E}_h $	h	E_u	$m(E_u)$	E_Γ	$m(E_\Gamma)$	
1	1	38	1.45e-01	2.72e-02	-	2.32e-03	-	
1	1	152	7.25e-02	7.18e-03	1.92	1.09e-03	1.09	
1	1	598	3.66e-02	1.91e-03	1.93	1.93e-04	2.53	
1	1	2392	1.83e-02	4.69e-04	2.03	3.92e-05	2.30	
2	2	38	1.45e-01	5.68e-03	-	4.83e-05	-	
2	2	152	7.25e-02	9.64e-05	5.88	2.70e-07	7.48	
2	2	608	3.63e-02	6.36e-06	3.92	1.20e-08	4.49	
2	2	2432	1.81e-02	8.66e-07	2.88	7.70e-10	3.96	
3	3	32	1.58e-01	1.57e-03	-	2.06e-05	-	
3	3	128	7.91e-02	1.62e-05	6.60	3.37e-07	5.93	
3	3	512	3.95e-02	4.37e-07	5.21	5.90e-09	5.84	
3	3	2040	1.98e-02	3.31e-08	3.73	1.87e-10	5.00	

Observation: Optimal convergence rates ($\mathcal{O}(h^{p+1})$) obtained for solution error; faster rates obtained for shock surface.