An Optimization-Based Discontinuous Galerkin Approach for High-Order Accurate Shock Tracking

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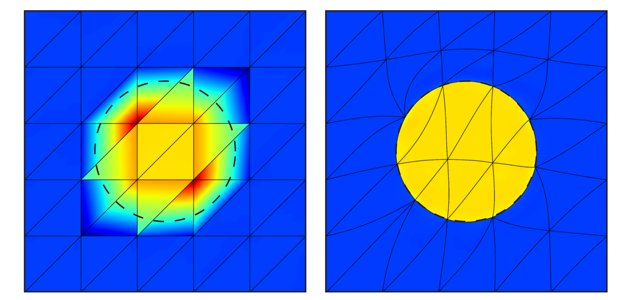
Abstract

We present a novel discontinuity-tracking framework for resolving discontinuous solutions of conservation laws with high-order discontinuous Galerkin methods [1, 2]. The proposed method aims to align the inter-element boundaries with discontinuities by deforming the computational mesh. A discontinuity-aligned mesh ensures the discontinuity is represented through inter-element jumps while smooth basis functions interior to elements are only used to approximate smooth regions of the solution, thereby avoiding Gibbs' phenomena that create well-known stability issues. Therefore, very coarse high-order discretizations accurately resolve the piecewise smooth solution throughout the domain. The method recasts the conservation law as a PDE-constrained optimization problem that simultaneously solves the conservation law and aligns the mesh with discontinuities. We demonstrate optimal $\mathcal{O}(h^{p+1})$ convergence rates and show that accurate solutions can be obtained on extremely coarse meshes.



Motivation and Impact

- Discontinuities and shape gradients arise in many important applications across engineering and sciences such as interfaces (multiphase flow, fluid-structure interaction) and shock waves (transonic and supersonic aerodynamics, hypersonic vehicle re-entry, explosion/implosion).
- However, the problem of finding (numerically) the solution of conservation laws when the solution contains discontinuities or sharp gradients has been a longstanding difficulty, particularly when high-order methods are used due to the smooth, high-order polynomial basis to represent the solution.
- Our method is designed to overcome these difficulties by simultaneously aligning the computational mesh with the discontinuities such that they can be exactly represented by the inter-element jumps without relying on the smooth, high-order basis.

High-order shock tracking framework

Governing equations and high-order numerical discretization

Consider a general system of conservation laws, defined on the physical domain $\Omega \subset \mathbb{R}^d$,

$$\nabla \cdot \mathcal{F}(U) = 0 \quad \text{in} \quad \Omega. \tag{1}$$

This could either represent a static conservation law on a d-dimensional spatial domain or a time-dependent conservation law on a $(d-1)$-dimensional spatial domain and the dth dimension is time, i.e., *a space-time formulation*. Discretization with a standard high-order nodal DG method in an arbitrary Lagrangian-Eulerian formulation yields

$$\boldsymbol{r}(\boldsymbol{u}, \boldsymbol{x}) = \boldsymbol{0}, \tag{2}$$

where the dependence on the discretize solution, $\boldsymbol{u}$, and coordinates of the mesh nodes, $\boldsymbol{x}$, is made explicit.

High-order discontinuity tracking via optimization-based r-adaptivity

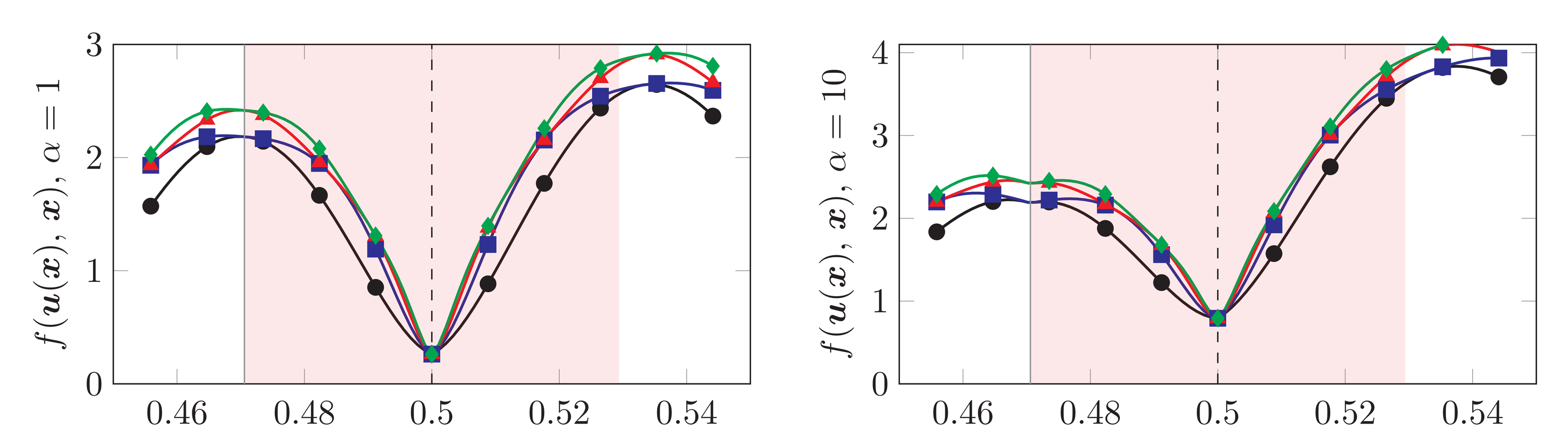
The proposed method for high-order resolution of discontinuous solutions of conservation laws reformulates the discrete nonlinear system in (2) as a PDE-constrained optimization problem that searches for the discrete solution, $\boldsymbol{u}$, and mesh, $\boldsymbol{x}$, that minimize some objective function and satisfy the discrete PDE

$$\begin{aligned} &\underset{\boldsymbol{u},\,\boldsymbol{x}}{\text{minimize}} \quad f(\boldsymbol{u}, \boldsymbol{x}) \\ &\text{subject to} \quad \boldsymbol{r}(\boldsymbol{u}, \boldsymbol{x}) = \boldsymbol{0}. \end{aligned} \tag{3}$$

For the proposed framework to successfully align faces of the computational mesh with discontinuities in the solution the objective function must 1) attain a local minimum at some discontinuity-aligned mesh and 2) monotonically decrease to such a minima is a neighborhood of radius approximately $h/2$. We define the objective function as

$$\begin{aligned} f(\boldsymbol{u}, \boldsymbol{x}) &= f_{shk}(\boldsymbol{u}, \boldsymbol{x}) + \alpha f_{msh}(\boldsymbol{x}) \\ f_{shk}(\boldsymbol{u}, \boldsymbol{x}) &= h_0^{-2} \sum_{K \in \mathcal{E}_{h,p}} \int_{\mathcal{G}(K,\boldsymbol{x})} \left|\left| u_{h,p} - \bar{u}_{h,p}^K \right|\right|_{\boldsymbol{W}}^2 \, dV \\ f_{msh}(\boldsymbol{x}) &= h_0^d \sum_{K \in \mathcal{E}_{h,p}} \frac{1}{|\mathcal{G}(K,\boldsymbol{x})|} \int_{\mathcal{G}(K,\boldsymbol{x})} \left(\frac{||G_{h,p}||_F^2}{(\det G_{h,p})_+^{2/d}} \right)^r. \end{aligned} \tag{4}$$

f_{shk} promotes transforming the mesh such that element faces align with discontinuities and f_{msh} ensures the mesh is well-conditioned.



The objective function for $\alpha = 1$ (*left*) and $\alpha = 10$ (*right*) as a function of 1D mesh deformation to show monotonicity of the objective function and it attains a minimum at the shock location (- - -) for DG elements with polynomial orders $p = 1$ (—●—), $p = 2$ (—■—), $p = 3$ (—▲—), $p = 4$ (—♦—).

Full space optimization solver and initialization

The final ingredient is the numerical solver for the PDE-constrained optimization problem in (3). Commonly used reduced space approaches *cannot be used because nonlinear instabilities will cause the CFD solver to crash and the mapping $\boldsymbol{u}(\boldsymbol{x})$ will not be defined*. Instead, we use a full space approach that directly solves (3), e.g., by finding a stationary point of the $\mathcal{L}(\boldsymbol{u}, \boldsymbol{x}, \boldsymbol{\lambda}) = f(\boldsymbol{u}, \boldsymbol{x}) - \boldsymbol{\lambda}^T \boldsymbol{r}(\boldsymbol{u}, \boldsymbol{x})$. A key feature of this approach is it never explicitly requires the solution of the nonlinear equations $\boldsymbol{r}(\boldsymbol{u}, \boldsymbol{x}) = 0$ (robustness issues), only its linearization

$$\boldsymbol{r}(\boldsymbol{u}_k, \boldsymbol{x}_k) + \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{u}}(\boldsymbol{u}_k, \boldsymbol{x}_k)\Delta \boldsymbol{u} + \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{x}}(\boldsymbol{u}_k, \boldsymbol{x}_k)\Delta \boldsymbol{x} = \boldsymbol{0}.$$

An initial guess for the optimization problem is generated by computing a *viscous* solution of the conservation law under consideration, i.e.,

$$\boldsymbol{r}_\nu(\boldsymbol{u}, \boldsymbol{x}) = \boldsymbol{0}, \tag{5}$$

where enough viscosity is added such that the solution can be reliably computed.

Results: 1D and 2D model problems

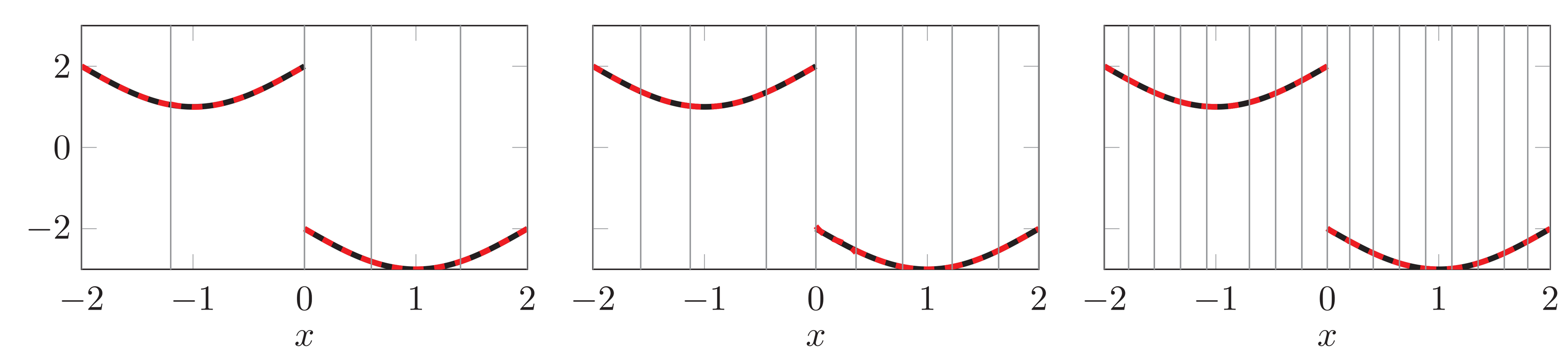
Inviscid Burgers' equation with discontinuous source term

Here, we present the shock tracking framework applied to the inviscid, modified one-dimensional Burgers' equation

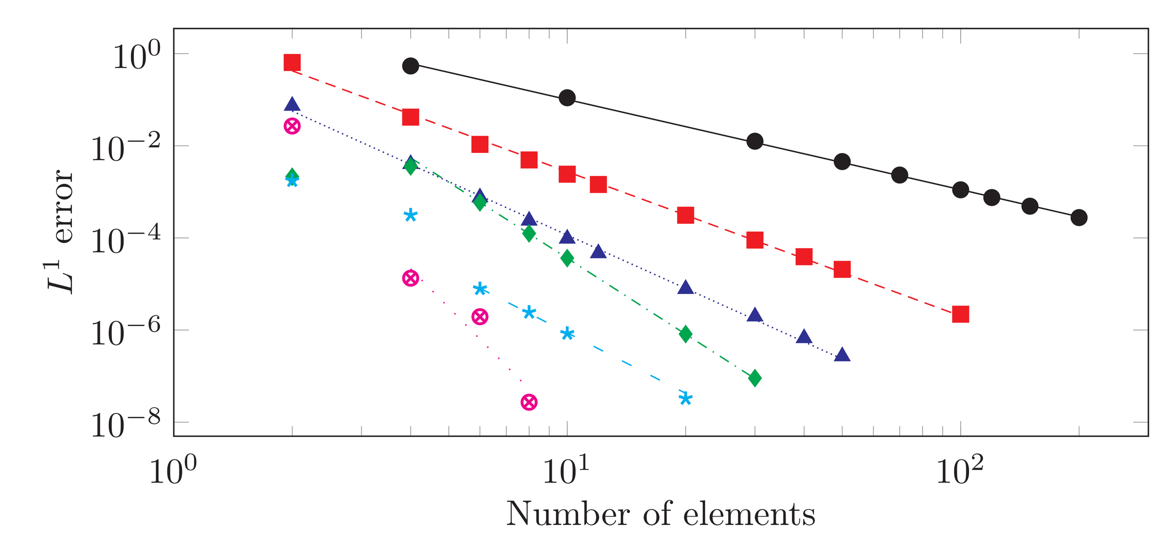
$$\frac{\partial}{\partial x}\left(\frac{1}{2}u^2\right) = \beta u + f(x), \quad \text{for } x \in \Omega \subset \mathbb{R},$$

where $\beta = -0.1$ and

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



Results of discontinuity-tracking framework applied to the solution of the inviscid Burgers' equation on a mesh with 5, 9, 17 (*left to right*) cubic elements. Legend: exact solution (▬▬) and solution obtained from tracking framework (——).

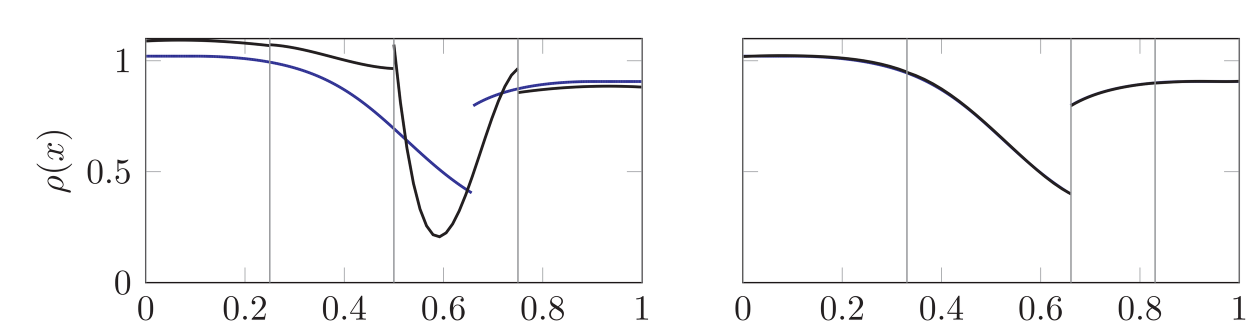


Convergence of tracking method applied to inviscid Burgers' equation for polynomial orders $p = 1$ (●), $p = 2$ (■), $p = 3$ (▲), $p = 4$ (♦), $p = 5$ (*), $p = 6$ (⊗). The expected convergence rates of $p+1$ are obtained in most cases. The slopes of the best-fit lines to the data points in the asymptotic regime are: $\angle -1.95$ (——), $\angle -3.13$ (- - - -), $\angle -3.85$ (·········), $\angle -5.47$ (-·-·-), $\angle -4.36$ (- -), $\angle -8.67$ (· · · ·).

Transonic, inviscid flow through nozzle

Our final one-dimensional example considers the relevant situation of transonic, inviscid flow through a converging-diverging nozzle. The quasi-one-dimensional Euler equations are used to model the inviscid, compressible flow in a variable-area stream tube $A(x)$

$$\frac{\partial}{\partial x}(A\rho u) = 0, \quad \frac{\partial}{\partial x}(A[\rho u^2 + p]) = \frac{p}{A}\frac{\partial A}{\partial x}, \quad \frac{\partial}{\partial x}(A[\rho E + p]u) = 0 \tag{6}$$



The solution of the quasi-1d Euler equations using 300 linear elements (——) and 4 quartic elements (——). *Left*: The high-order elements are not aligned with the shock and cause substantial over/under-shoot. *Right*: The high-order DG shock tracking framework is applied to align the high-order elements with the shock and the resulting solution matches the 300 element reference solution very well, with substantially fewer degrees of freedom.

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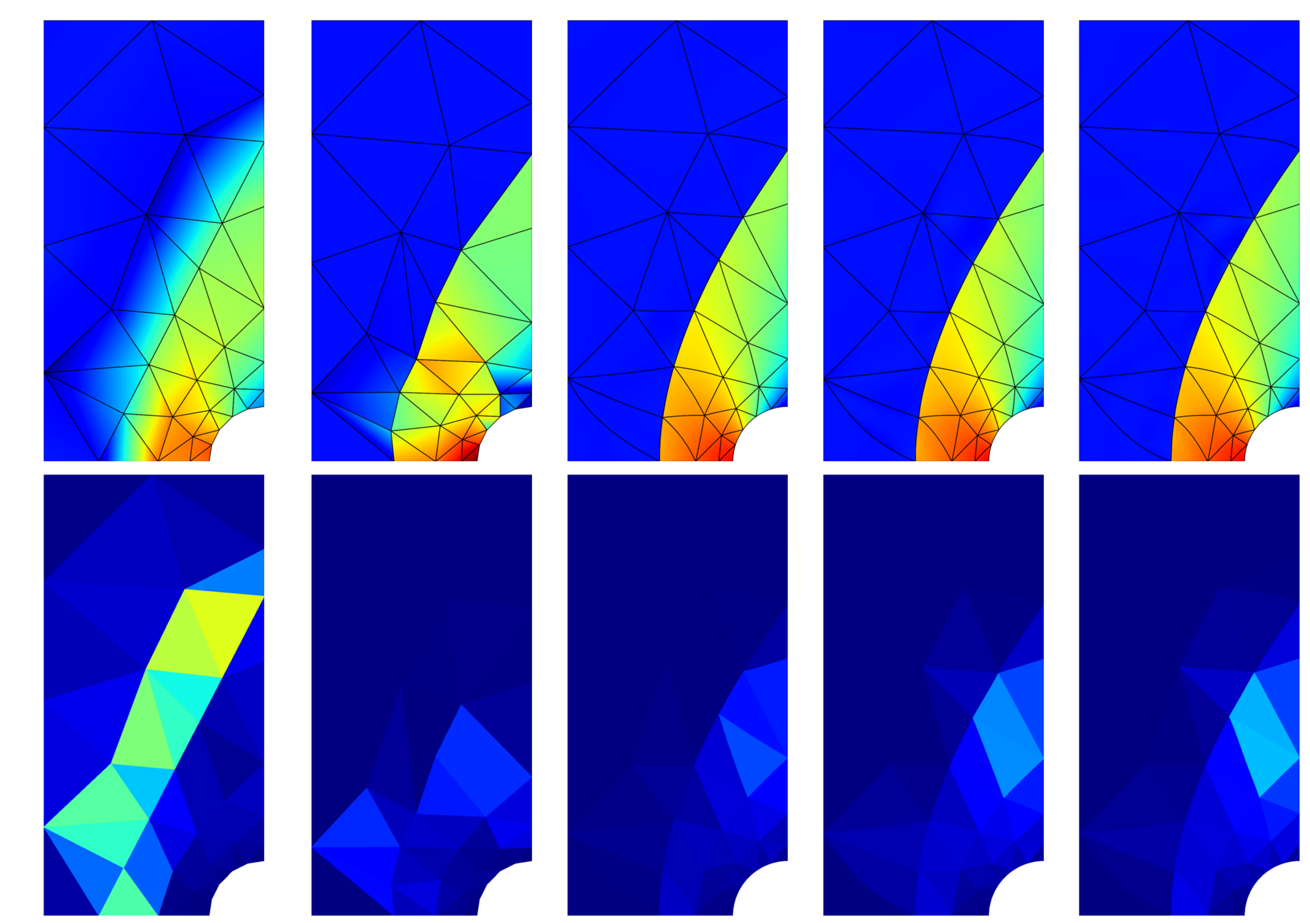
Supersonic flow around 2D cylinder

Finally, we demonstrate the shock tracking framework on the relevant problem of supersonic ($M = 2$) flow around a cylinder, modeled using the 2D Euler equations. For convenience, only 1/4 of the domain is modeled.

$$\frac{\partial}{\partial x_j}(\rho u_j) = 0, \quad \frac{\partial}{\partial x_j}(\rho u_i u_j + p) = 0, \quad \frac{\partial}{\partial x_j}(u_j(\rho E + p)) = 0.$$



Solution of supersonic flow around cylinder using shock shocking framework (*top*) and elementwise shock indicator, $f_{shk}(\boldsymbol{u}, \boldsymbol{x})$ (*bottom*). *Columns, left-to-right*: viscosity solution on the non-aligned $p = 1$ mesh and the inviscid solution with shock tracking method with $p = 1, 2, 3, 4$ elements.

Polynomial order (p)	1	2	3	4
Degrees of freedom ($N_{\boldsymbol{u}}$)	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
Number of optimization iterations	396	283	103	121

Synopsis of my contributions

- Moved prototyped Python implementation into scalable C++ implementation, which enabled easier parallel implementation and usage of sparse-data structures.
- Implemented the idea of 'space-time' problem solving using the existing steady-state framework in [1].
- Computed the exact derivatives of the objective function for optimization, instead of approximating using finite differences, leading to better accuracy.

Conclusions and Future work

- The introduced framework was tested on various 1D and 2D problems. The objective function is succesful in aligning the computational mesh with the discontinuities.
- Also the objective function attained a local minimum at the discontinuity.
- The optimization problem is solved using a full-space optimizer, which is highly effective for our setting, than the reduced-space solvers.
- Next, we intend to use more-refined parallelism, and exploit the sparsity of the Jacobians of the residual to increase the efficiency.
- After successfully implementing the 1D spacetime idea, we next aim to tackle the 2D and 3D problems.

References

[1] Matthew J. Zahr and Per-Olof Persson. An optimization-based discontinuous Galerkin approach for high-order accurate shock tracking. In *AIAA Science and Technology Forum and Exposition (SciTech2018)*, Kissimmee, Florida, 1/8/2018 – 1/12/2018. American Institute of Aeronautics and Astronautics.

[2] Matthew J. Zahr and Per-Olof Persson. An optimization-based approach for high-order accurate discretization of conservation laws with discontinuous solutions. *Journal of Computational Physics*, 365:105 – 134, 2018.