An optimization-based discontinuous Galerkin approach for high-order shock tracking

Matthew J. Zahr[†] and Per-Olof Persson

5th International Workshop on High Order CFD Methods
Test Case: CI1 - Inviscid Bow Shock
Gaylord Palms, Kissimmee, Flordia
January 6, 2018

[†] Luis W. Alvarez Postdoctoral Fellow
Department of Mathematics
Lawrence Berkeley National Laboratory

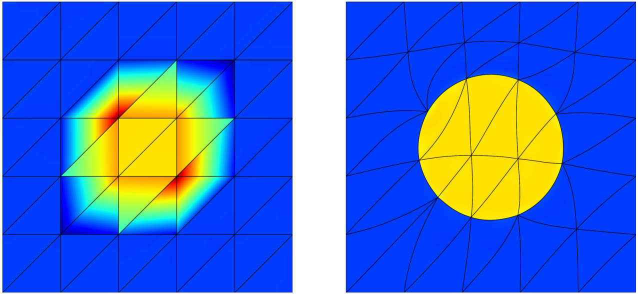
BERKELEY LAB

Proposed shock tracking method

- Key observation

  in a discontinuous Galerkin or finite volume setting, if (curved) face of an element is perfectly aligned with the (unknown) shock, the Riemann solver will provide appropriate stabilization and allow for high-order approximations of the solution on both sides of the discontinuity

- Propose a PDE-constrained optimization framework to simultaneously align mesh with shock and solve discrete PDE



Non-aligned (*left*) vs. discontinuity-aligned (*right*) mesh and corresponding solution

Shock tracking optimization formulation

- Consider the spatial discretization of the conservation law

$$\nabla \cdot \mathcal{F}(U(x)) = 0, \quad x \in \Omega \qquad \rightarrow \qquad \boldsymbol{r}(\boldsymbol{u}, \boldsymbol{x}) = \boldsymbol{0}$$

  - U, x are the conservation law state vector and domain coordinate
  - $\boldsymbol{x}$ contains the coordinates of the *continuous*, *high-order* mesh nodes
  - $\boldsymbol{u}$ contains the discrete state vector corresponding to U at the mesh nodes
- Fundamental requirement on discretization: basis supports discontinuties along element **faces**, i.e., **discontinuous Galerkin**, finite volume
- Shock tracking formulation

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

Shock tracking objective function

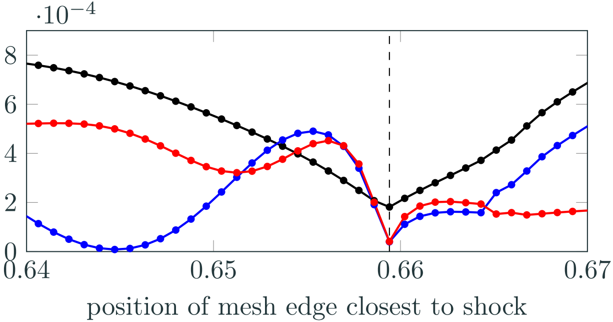
Requirements on objective function

obtains minimum *when mesh face aligned with shock and* ***monotonically*** *decreases to minimum in (large) neighborhood*

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

$$f_{shk}(\boldsymbol{u}, \boldsymbol{x}) = \sum_{e=1}^{n_e} \int_{\Omega_e(\boldsymbol{x})} \left|\boldsymbol{u} - \bar{\boldsymbol{u}}_e\right|^2 \, dV$$

$$f_{msh}(\boldsymbol{x}) = \sum_{e=1}^{n_e} \int_{\Omega_e(\boldsymbol{x})} \frac{||\boldsymbol{G}||_F^2}{(\det \boldsymbol{G})_+^{2/d}}$$



Objective function as an element edge is smoothly swept across shock location for: $f_{shk}(\boldsymbol{u}, \boldsymbol{x})$ (black), residual-based objective (blue), and Rankine-Hugniot-based objective (red).

Full space optimization solver for shock tracking

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

- **Full space approach**: $\boldsymbol{u} \rightarrow \boldsymbol{u}^*$ and $\boldsymbol{x} \rightarrow \boldsymbol{x}^*$ *simultaneously*
- Define Lagrangian

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

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

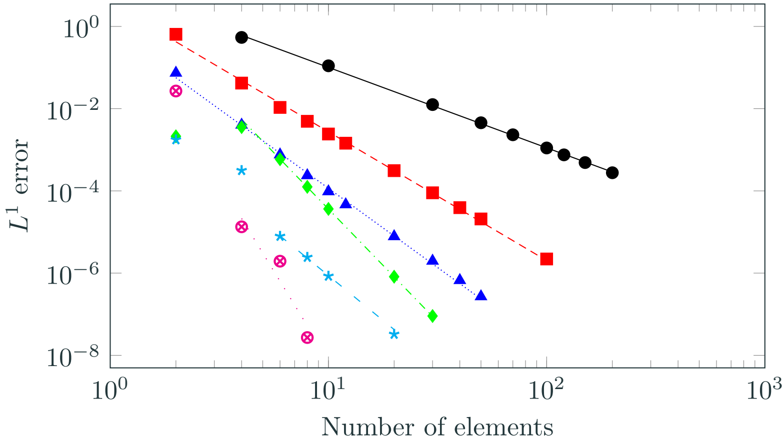
$$\nabla_{\boldsymbol{u}} \mathcal{L}(\boldsymbol{u}^*, \boldsymbol{x}^*, \boldsymbol{\lambda}^*) = \mathbf{0}, \qquad \nabla_{\boldsymbol{x}} \mathcal{L}(\boldsymbol{u}^*, \boldsymbol{x}^*, \boldsymbol{\lambda}^*) = \mathbf{0}, \qquad \nabla_{\boldsymbol{\lambda}} \mathcal{L}(\boldsymbol{u}^*, \boldsymbol{x}^*,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

- Apply (quasi-)Newton method[1] to solve nonlinear KKT system for $\boldsymbol{u}^*, \boldsymbol{x}^*, \boldsymbol{\lambda}^*$
- SNOPT used in this work[2]

[1] usually requires globalization such as linesearch or trust-region

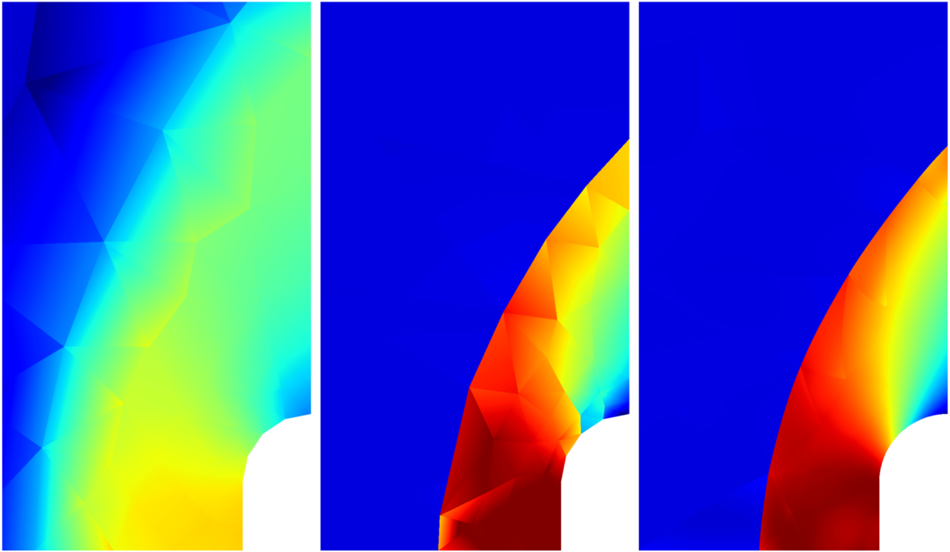
[2] leads to very inefficient implementation since cannot leverage data structures from DG discretization and cannot be parallelized

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



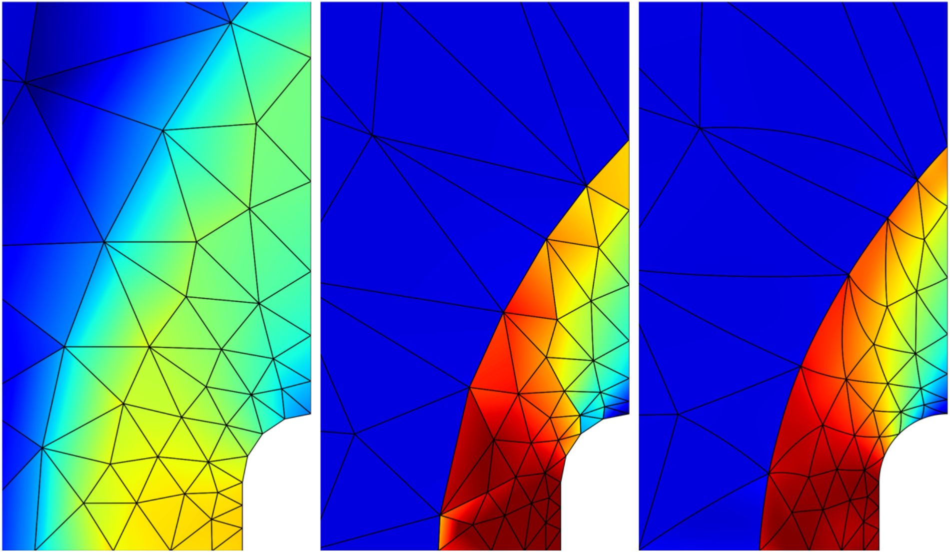
Convergence of shock tracking method applied to the modified inviscid Burgers' equation for polynomial orders $p = 1$ (●), $p = 2$ (■), $p = 3$ (▲), $p = 4$ (♦), $p = 5$ (*), $p = 6$ (⊗). The expected convergence rates of $p + 1$ are obtained in most cases. The slopes of the best-fit lines to the data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

Resolution of 2D supersonic flow with 102 quadratic elements



The solution of the CI1 bow shock problem. *Left*: Solution 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.

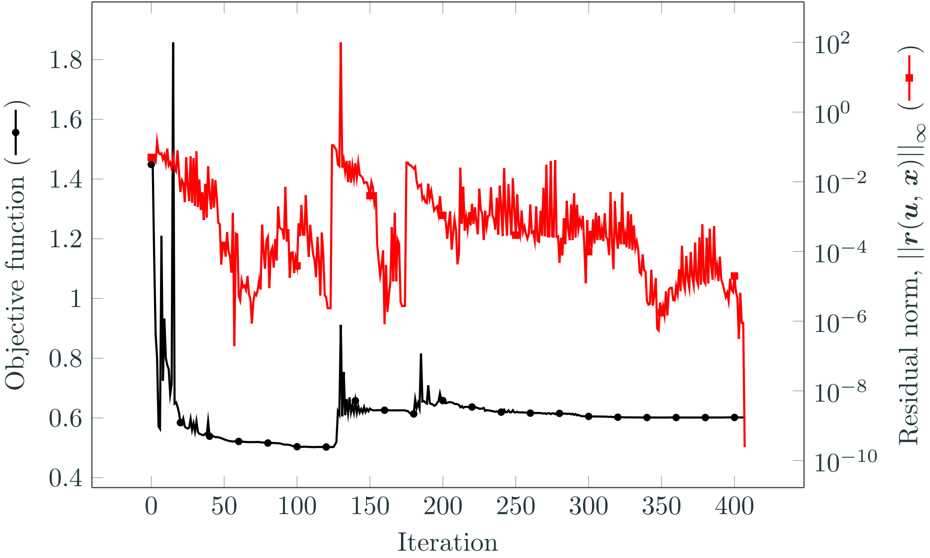
Resolution of 2D supersonic flow with 102 quadratic elements



The solution of the CI1 bow shock problem. *Left*: Solution 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

Performance summary for shock tracking method

Polynomial order (p)	2
Number of elements	102
Degrees of freedom	2448
Enthalpy error (normalized)	0.000694 (0.0111)
Stagnation pressure error (normalized)	0.0681 (1.09)
Cost (tau bench)	22.8

Shock tracking performance summary for mesh with 102 elements and polynomial orders $p = 1$ and $p = 2$ with mesh regularization $\alpha = 0.05$.

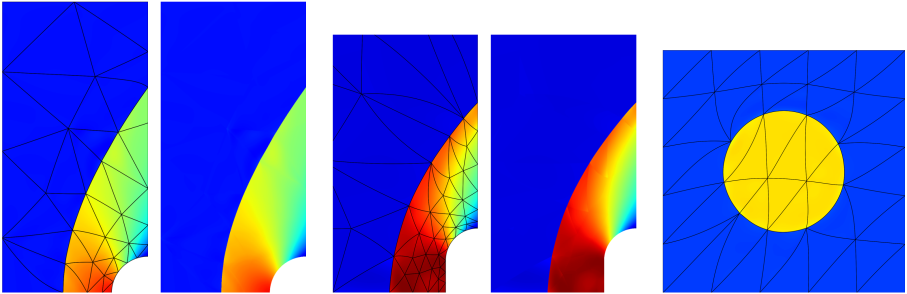
BERKELEY LAB

Conclusions

Matthew J. Zahr and Per-Olof Persson, "An optimization-based discontinuous Galerkin approach for high-order accurate shock tracking.", *Monday, January 8, 2018, 10:00AM-10:30AM, Sun 5 Room.*

Upcoming improvements to method

- **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
- **parallel** implementation



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

References I

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. (2018a).
An optimization-based approach for high-order accurate discretization of conservation laws with discontinuous solutions.
In review.