2-D Shock AD

Practical Difficulties and (Im-) Practical Solutions

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08.12.2025

Software and Tools for Computational Engineering
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Conservation Laws

Integral and Differential Form[4]

Given time $t \in \mathbb{R}^+$ and space coordinate $\vec{x} \in \Omega \subset \mathbb{R}^{n_d}$, a conservation law (usually) has the form:

$$\partial_t U + \operatorname{div}_x F(U) = 0 \tag{1}$$

or, perhaps more usefully:

$$\frac{d}{dt} \int_\Omega U \, dx + \oint_{\partial\Omega} F(U) \, \hat{n} \cdot dS = 0$$

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- Solutions to conservation laws can exhibit discontinuities, even if $U(0, x)$ is smooth!
- Conservation laws are also *hyperbolic PDEs* iff $\nabla_U F$ is diagonalizable with real eigenvalues.
- We (usually) solve (systems of) conservation laws using finite volume methods.

Conservation Laws

Discretizing a Conservation Law

1. Choose a set of time levels $0 = t_0 < t_1 < \ldots < t_n < T$.
2. Decompose the space domain V into a set of cells C_j, for which the *cell-averaged value* of U is computed:

$$\bar{U}_j(t) = \int_{C_j} U(t, x)\, dA \tag{2}$$

3. Choose a time-stepping method for the cell-averaged values $\bar{U}_j$. Flux-differencing and finite-difference methods are of practical interest.
   - Godunov's Method (1D) *(monotone, nonlinear)*

$$\bar{U}_j(t_{n+1}) = \bar{U}_j(t_n) + \frac{1}{\Delta x} \int_{t_n}^{t_{n+1}} \tilde{F}_{tot}(\bar{U}) \tag{3}$$

   - Lax-Friedrichs (1D) *(linear)*

$$\bar{U}_j(t_n + 1) = \frac{1}{2} \left(\bar{U}_{j-1}(t_n) + \bar{U}_{j+1}(t_n)\right) + \frac{\Delta t}{2\Delta x} \left(F(\bar{U}_{j-1}(t_n)) - F(\bar{U}_{j+1}(t_n))\right) \tag{4}$$

Differentiating the Discretization

Accumulating tangents or adjoints of a time-stepping procedure is simple[1].

- Tangent update of a flux-differencing scheme w.r.t parameters at $t = t_0$:

$$U_i^{(1)}(t + \Delta t) = U_i^{(1)}(t) + \frac{\Delta t}{\Delta x}\left(\nabla_U \tilde{F}_{i-\frac{1}{2}}\, U^{(1)}(t) - \nabla_U \tilde{F}_{i+\frac{1}{2}}\, U^{(1)}(t)\right) \tag{5}$$

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- Is differentiating the discretization the same as discretizing the tangent or adjoint equations?
- Are there any dangers lurking behind these update rules?

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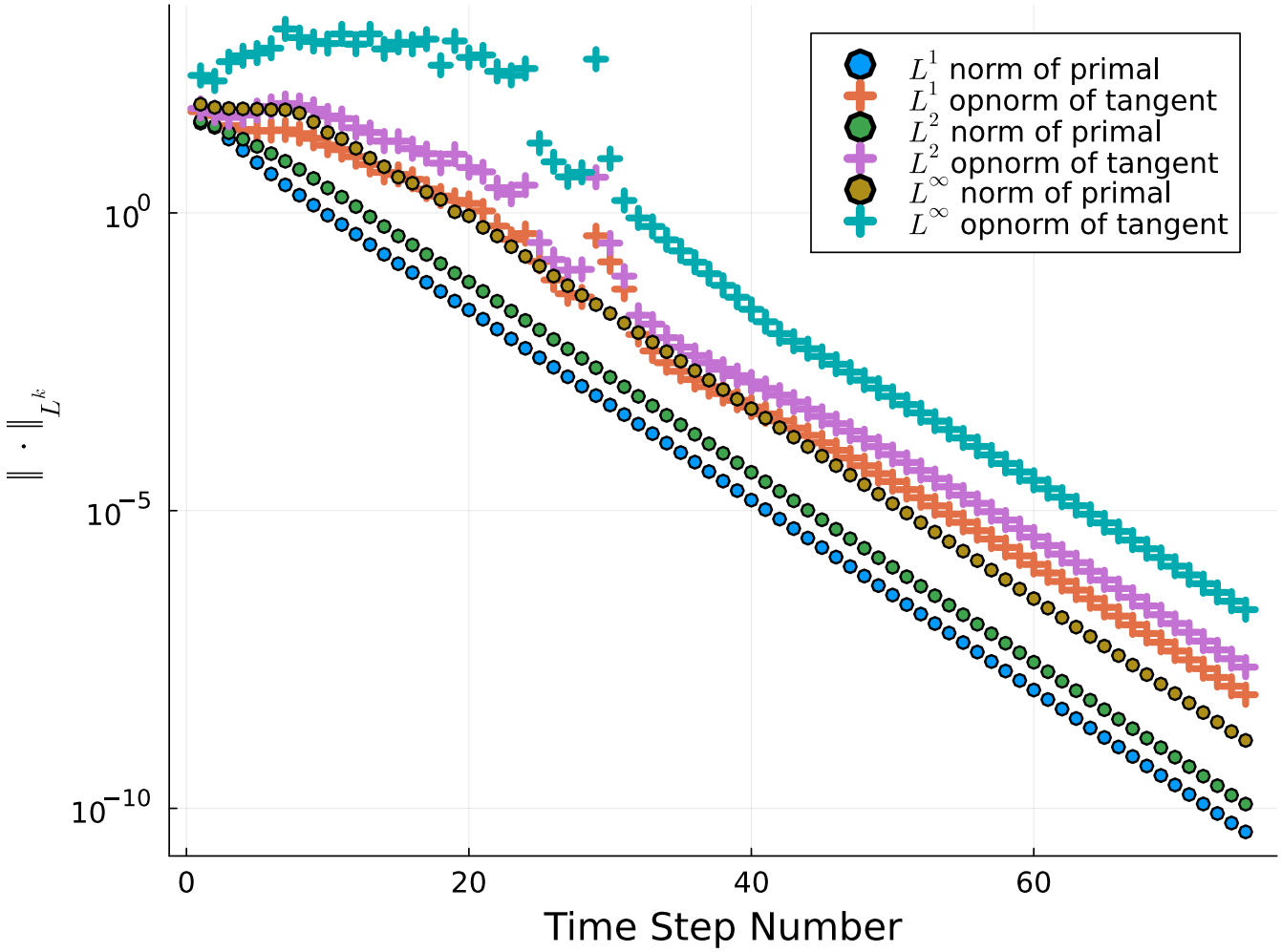
Conservation Laws



Existing Work

Burgers Equation

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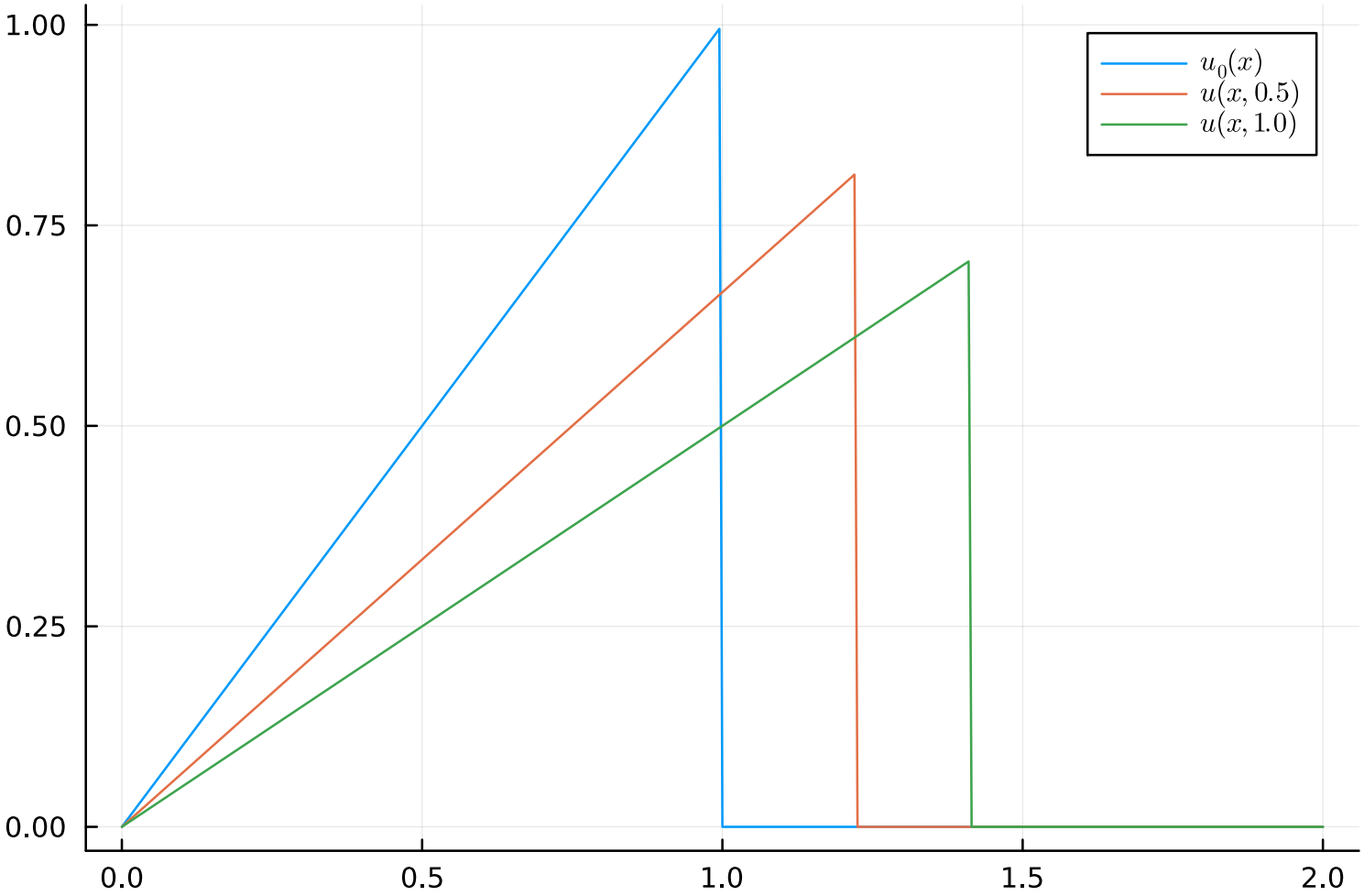
- A "simple" PDE that develops discontinuities if the initial data is not monotonically increasing.
- The flux function $f(u) = \frac{1}{2}u^2$ is cheap to compute.
- The Jacobian of the flux function has one eigenvalue.

An Example[2]

$$u(x, 0) = (1 + \varepsilon)x * \mathcal{X}_{[0,1]}(x)$$
$$u(x, t) = \frac{(1 + \varepsilon)x}{1 + (1 + \varepsilon)t} * \mathcal{X}_{[0,\sqrt{1+(1+\varepsilon)t}]}(x)$$

Existing Work



Existing Work

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First-order Approximations[2]

For a solution to a system of conservation laws $\vec{u}(t, x)$ with k discontinuities, a *generalized tangent vector* $(\vec{v}, \xi_k)$ induced by a perturbation ε is

$$\vec{u}^{\varepsilon}(x) = \vec{u}(x) + \varepsilon \vec{v}(x) + \sum_k \left(\vec{u}_R(x_k) - \vec{u}_L(x_k)\right) \mathcal{X}_{[x_k, x_k + \varepsilon \xi_k]}(x) \tag{7}$$

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- In this case, $\varepsilon\vec{v}(x)$ is the first term in the Taylor expansion of u.
- $\varepsilon\xi_k$ is the sensitivity of the shock wave position to the initial conditions.

Existing Work

In his dissertation, Hüser developed a method for computing these GTVs by augmenting the time stepping scheme with an additional ODE derived from the Rankine-Hugoniot conditions.

- This method requires estimates for the solution $\bar{u}$ and accumulated tangents *barv*.
- This method also requires esimates for the shock sensitivity and location.

Another Classic Example

Euler Equations

The Euler equations describe the evolution of density (ρ), momentum density ($\rho\vec{v}$), and total internal energy density (ρE) of an inviscid gas.

$$\begin{aligned} \partial_t \rho + \operatorname{div} \rho\vec{v} &= 0 \\ \partial_t \left(\rho\vec{v}\right) + \operatorname{div} \left(\rho\vec{v} \otimes \vec{v} + \mathbf{I}P\right) &= 0 \\ \partial_t \left(\rho E\right) + \operatorname{div} \left(\vec{v} \cdot \left(\rho E + P\right)\right) &= 0 \end{aligned} \tag{8}$$

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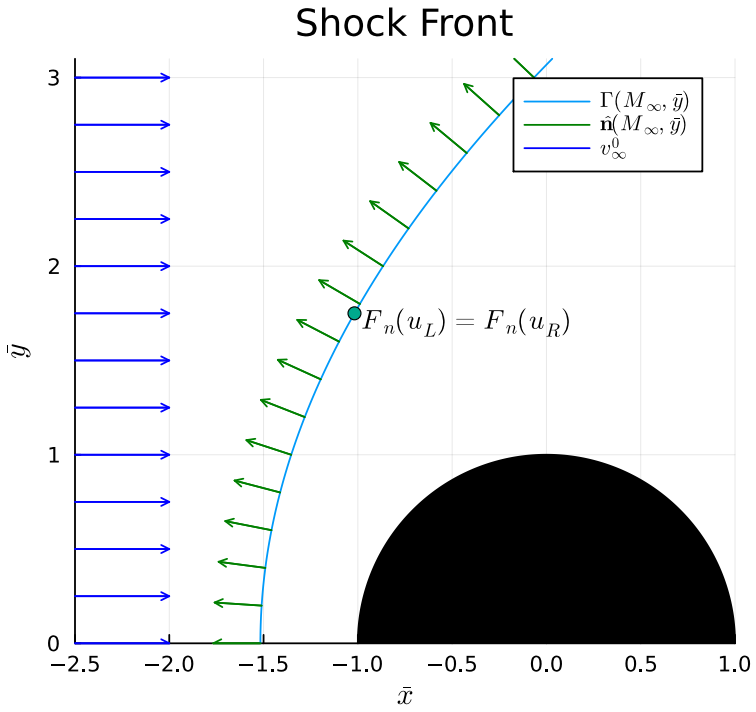
- We denote divergence of a vector field via the div operator.
- $\mathbf{I}$ denotes the identity matrix of the appropriate size.
- $\otimes$ denotes the vector outer product $u_{ij} = v_i w_j$

Extending to Two Dimensions



- Gas traveling at $M > 1$ flows past a blunt body centered at the origin.
- A shock front will develop, and the system will reach a steady state (given appropriate boundary conditions).
- Adjusting the free-stream flow parameters will change the location of the shock.

Extending to Two Dimensions

What is required to extend the generalized tangent vector formulation to solutions of the bow-shock problem?

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Broad Tangent V

The broad tangent V is simply the accumulated cell-average tangents in each cell. Perturbing the simulation parameters by ε would then yield the first order variation:

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- We know that there are shocks involved, however, and that this is not the final object we wish to compute.
- However, this expansion is perfectly valid (far) away from any shocks.

Extending to Two Dimensions

2-D Shock Curve $\Gamma(w)$

In the bow-shock problem, we know there is one detached shock.

- This shock curve is parametrizable by some parameter w.
- $\Gamma(w)$ does not form loops or have holes.

We would like there to be an equivalent to $\xi(t, x_k)$ from the one-dimensional example that yield this expansion of the shock curve:

$$\Gamma(w; p + \varepsilon) \approx \Gamma(w; p) + \xi(w)\varepsilon\hat{n}(w)$$

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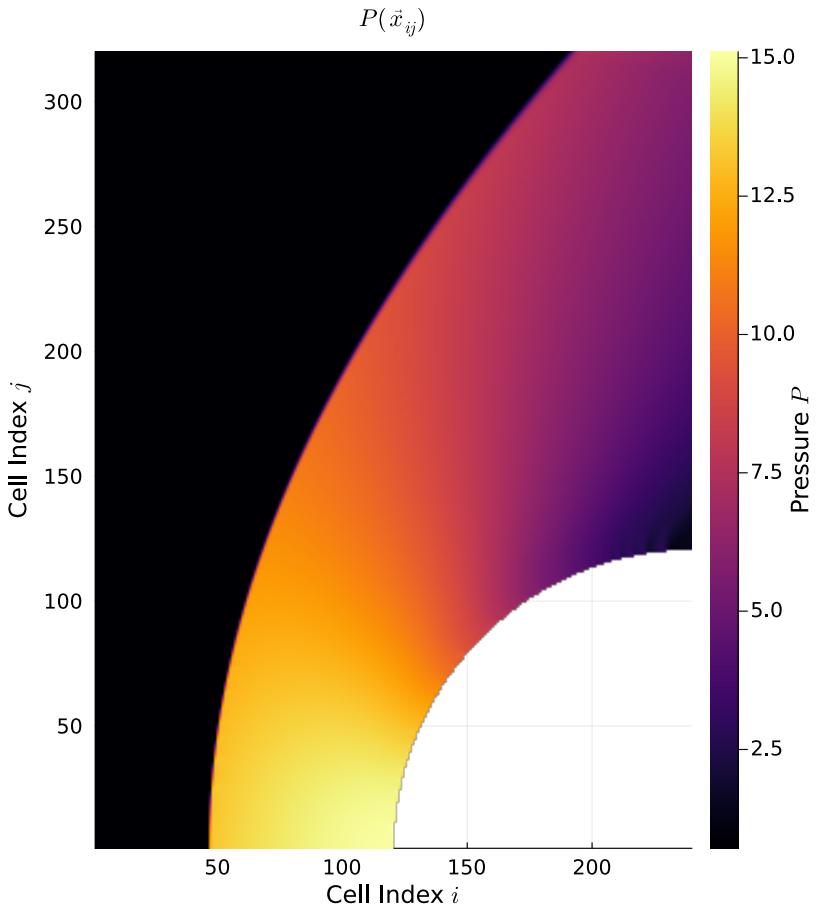
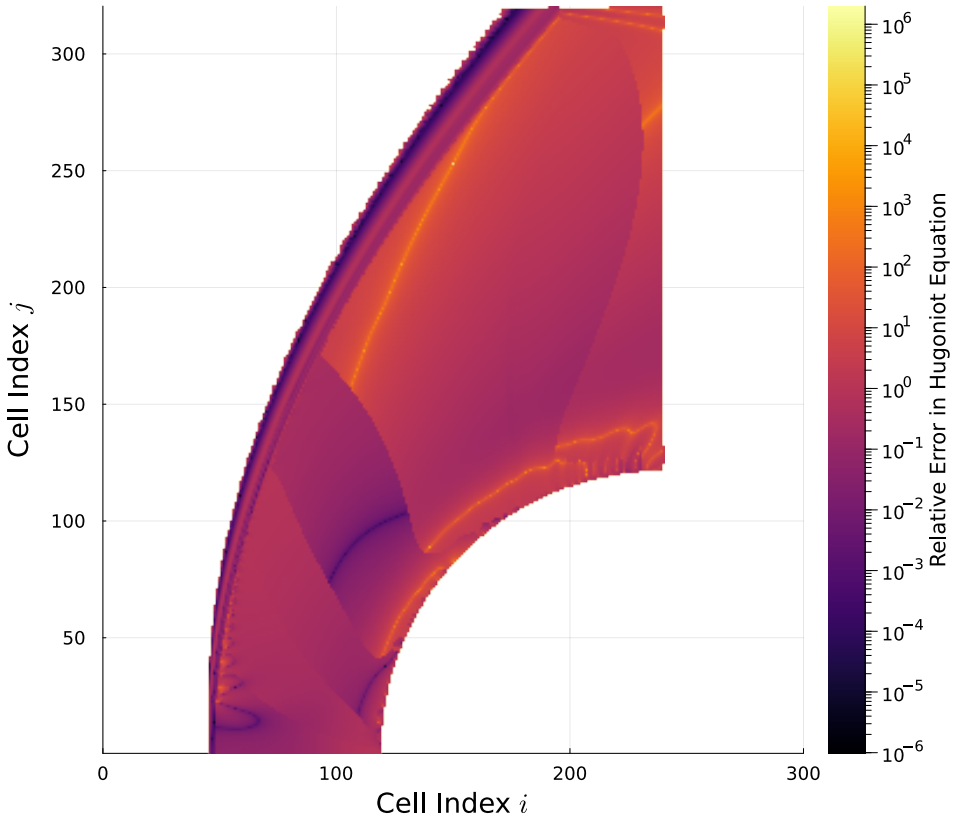
- This form makes sense; if the shock is moving, it propagates in a direction normal to itself.
- This expansion makes it somewhat more difficult to write the full GTV expansion in a neat way, but it is *possible* to do so.

Extending to Two Dimensions



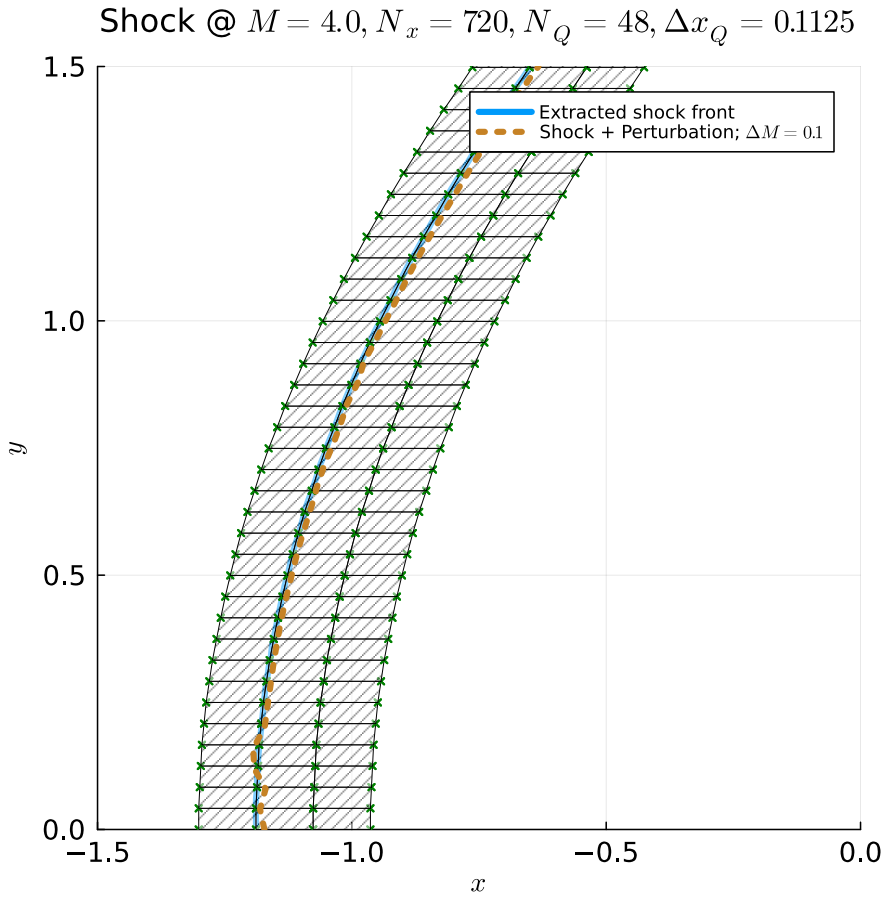
- The Euler Equations can be solved with a finite volume discretization.
- The 2nd space dimension can be handled via Strang splitting.
- Figure to the left is the pressure field $P(x; p)$

Extending to Two Dimensions



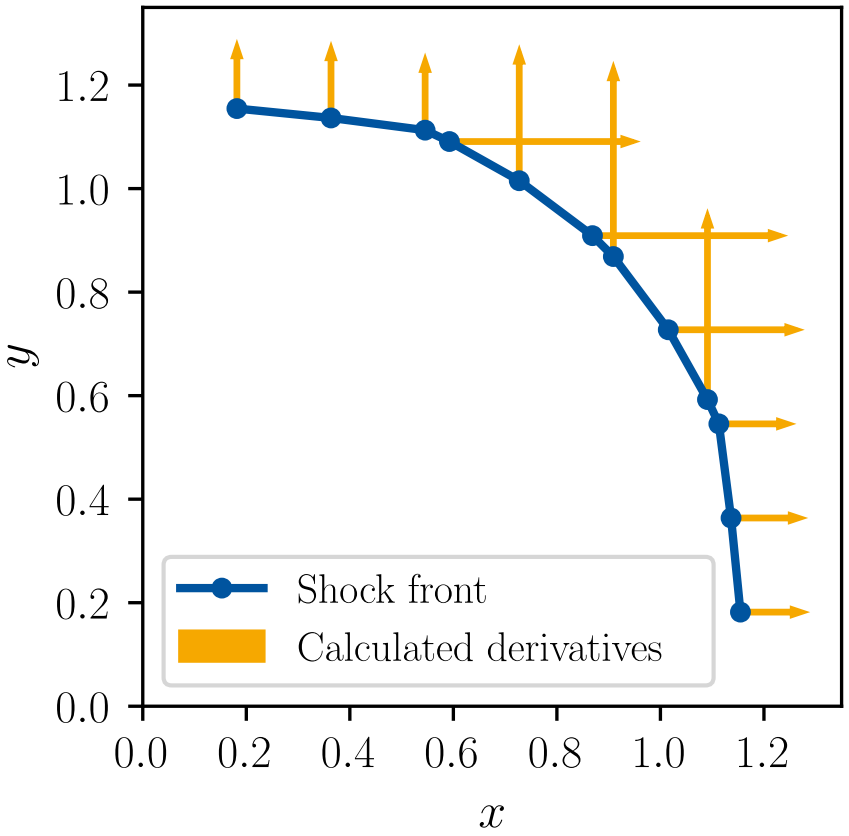
- We can extract the shock location by using Canny edge-detection[3].
- The figure to the left shows the relative error in the Hugoniot equation, which holds true for *admissible* discontinuities.

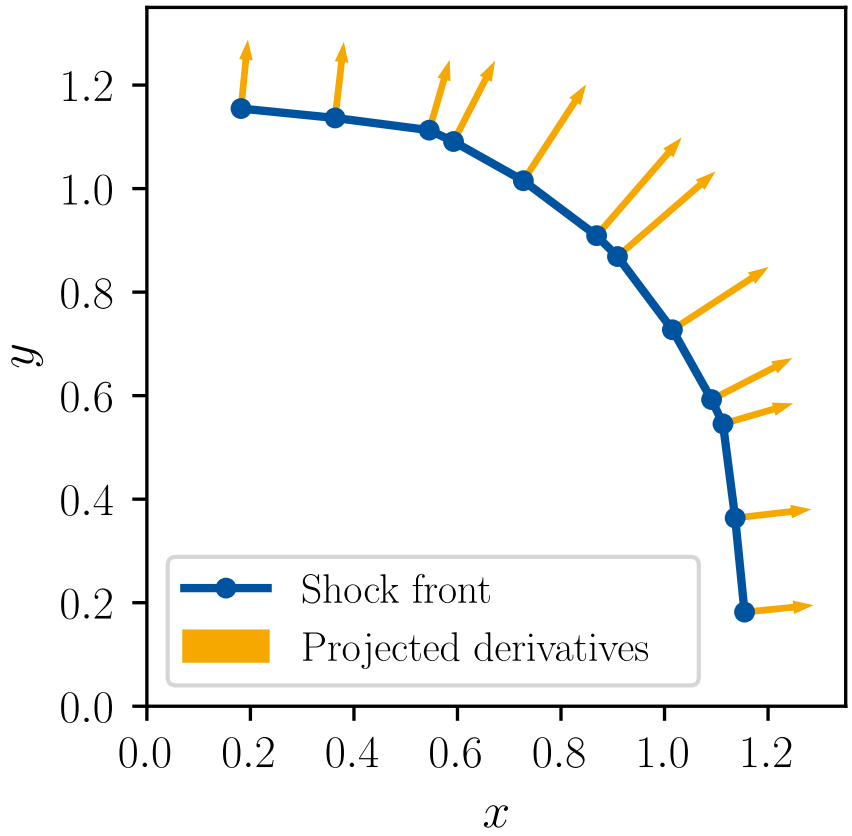
Extending to Two Dimensions



- The extracted shock can be used to compute the shock sensitivities.
- The figure to the left shows the shock extracted from a simulation of the bow-shock problem and its predicted shift, if the Mach number were increased by $\Delta M = 0.1$.

Naïve AD Yields Lovecraftian Horror





Shock propagation is limited to axial directions.[1]

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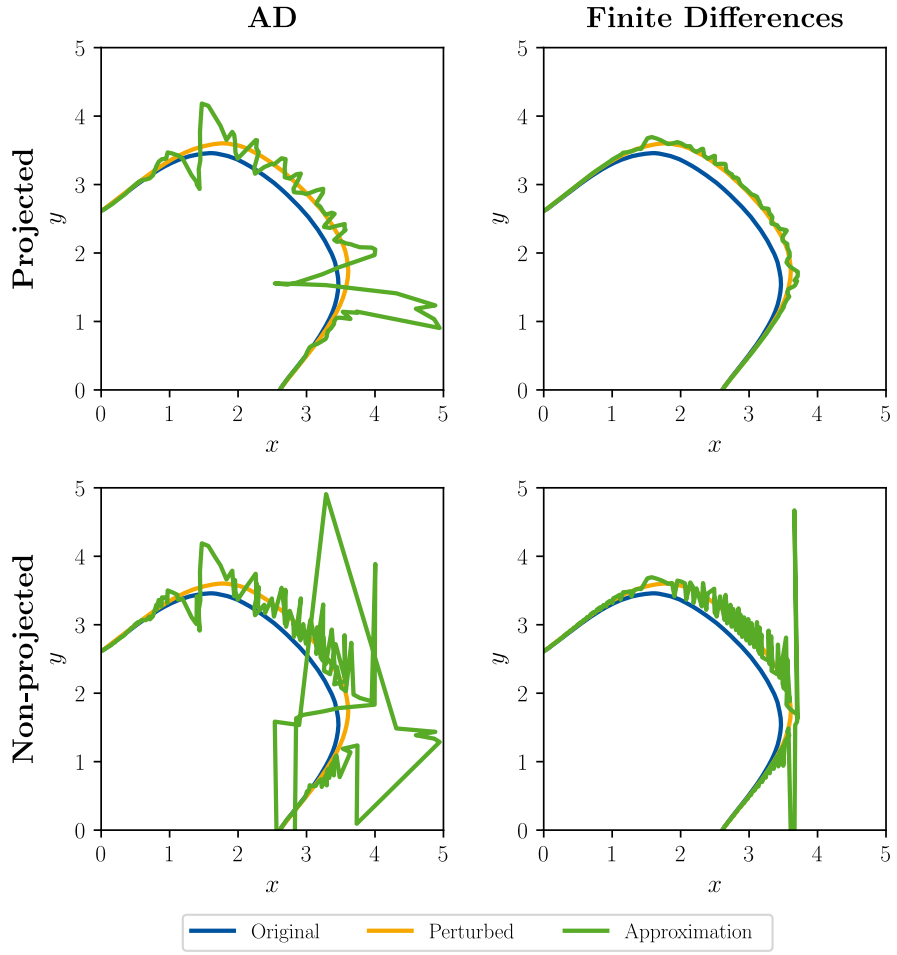

Oh no.[1]

Can we save ourselves?

Steady-State Bow Shocks

Let's choose an arbitrary control volume Q_i. Since we are interested in steady-sate solutions to the bow-shock problem, we (clearly?) have:

$$\partial_t \int_{Q_i} U \, dx = 0 = \oint_{\partial Q_i} F(U) \, \hat{n} \cdot dS$$

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Picking a Particular Q_i

Why not pick a set of control volumes where the previous boundary integral is easy[2] to compute? If Q_i is a set of convex polygons...

$$\oint_{\partial Q_i} F(U) \, \hat{n} \cdot dS = \sum_{\partial Q_i = k \text{ edges of } Q_i} F(U^{\downarrow}(\partial Q_{i,k})) \, L(\partial Q_{i,k}) \cdot \hat{n}(\partial Q_{i,k})$$

[2] citation needed.

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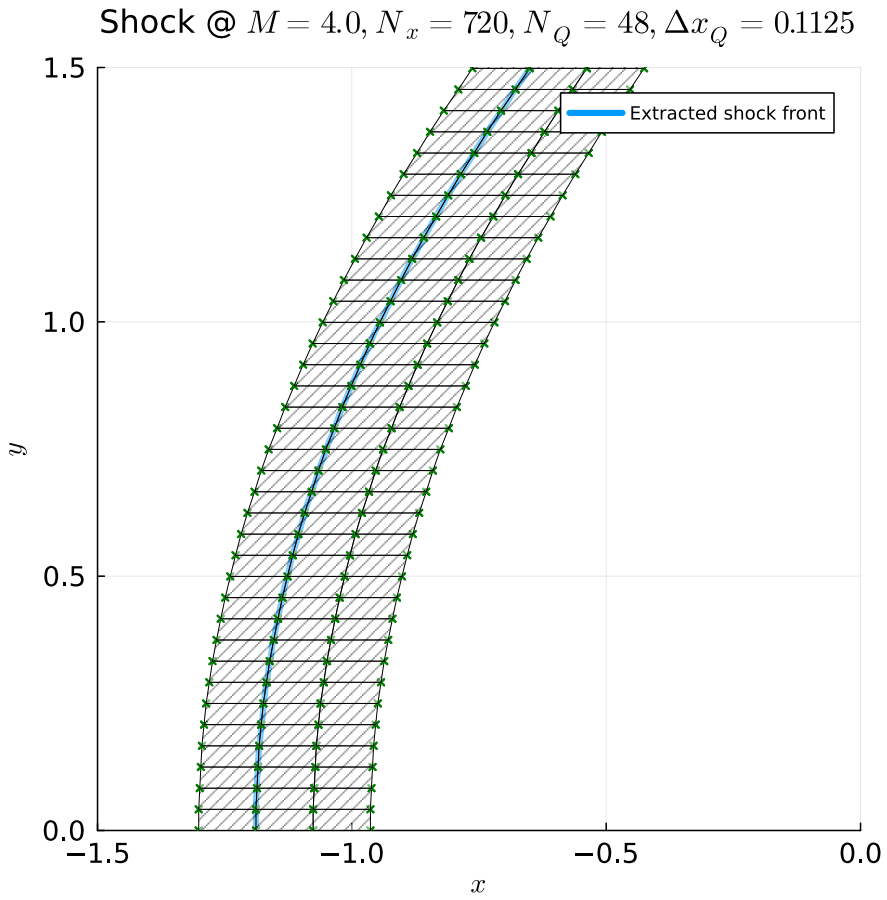

- We don't need very many cells for our intended purpose...
- We can also (ab-) use boundary conditions to save even more effort later.

Can we save ourselves?

Shock AD Mission Plan

1. Choose the control volumes Q_i such that some number of them share an edge that is on a linear interpolation of the shock.
2. Then, Q_i and their boundaries depend on the shock shifts s_k!
3. Compute the average value and tangent of U inside the control volumes Q_i.
4. Use a variant of the implicit function theorem to find the relationship between s_k and the parameters p.

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- Executing the mission plan requires some executive decision-making.
- Which derivatives do we have? Which derivatives do we need? Do we have error estimates?

A Hindrance to Saving Ourselves

Computing $\bar{U}_i$

$$\begin{aligned}\bar{U}_i &= \frac{1}{|Q_i|}\sum_j \iint_{C_j \cap Q_i} u(x)\,dA \\ &= \frac{1}{|Q_i|}\sum_j \iint_{C_j \cap Q_i} \bar{U}_j + \nabla_x U(x - x_{c,j})\,dA\end{aligned}$$

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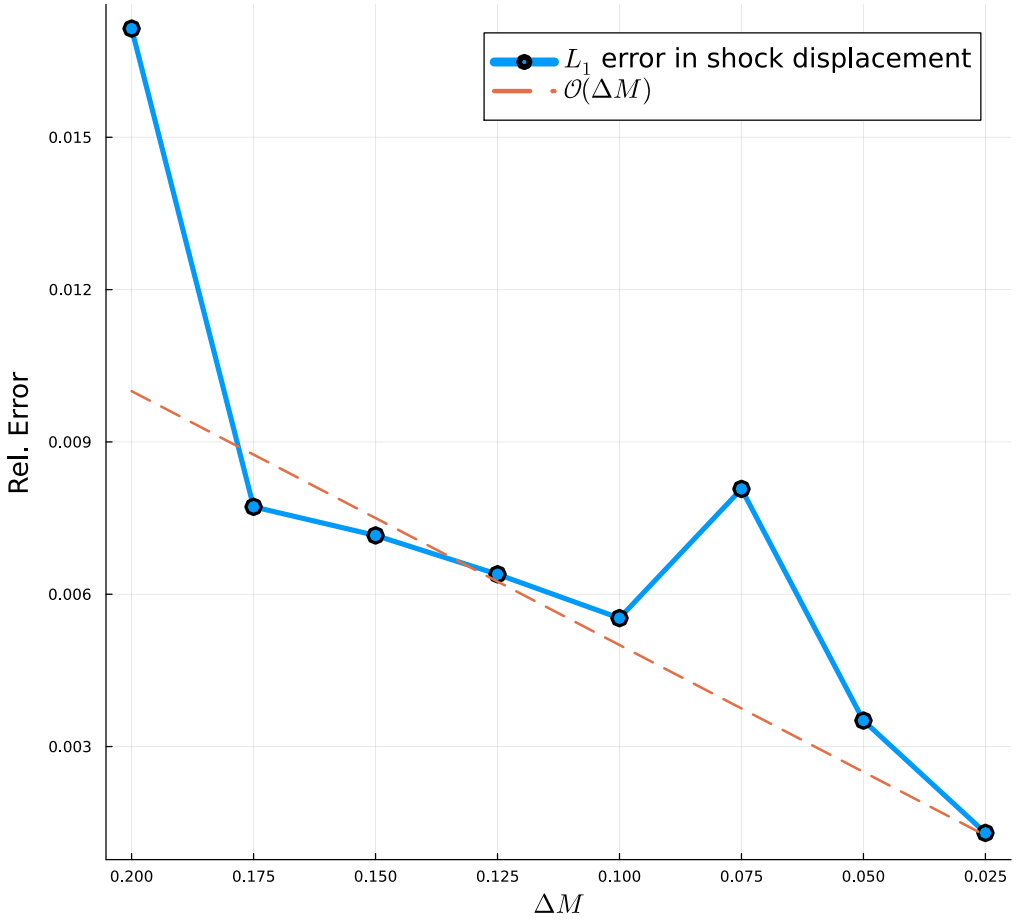
- That gradient strikes fear into our hearts; if we do not have an $\mathcal{O}(\Delta x^2)$ estimate for it, we might completely fail to compute the shock sensitivities.
- Even if we do, the gradient is relevant *near* to the shock; if the backing numerical method produces oscillations, we can't accurately compute *any* gradients near the shock.

Does it work?

Well...

Does it work?

$$N_{x,\,sim} = 720,\ N_Q = 48,\ \Delta x_Q = 0.075,\ \frac{V_Q}{V_{sim}} \approx 719.25$$



Accessing this Research

Much of my code is available here...

`https://github.com/STCE-at-RWTH`

References

[1] Gidon Bauer. "Differentiating Shocks in the Two-Dimensional Burgers Equation". MA thesis. RWTH Aachen University, Feb. 2025.

[2] Alberto Bressan and Andrea Marson. "A Variational Calculus for Discontinuous Solutions of Systems of Conservation Laws: A Variational Calculus for Discontinuous Solutions". In: *Communications in Partial Differential Equations* 20.9-10 (Jan. 1995), pp. 1491–1552. ISSN: 0360-5302, 1532-4133. DOI: 10.1080/03605309508821142.

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