# Numerical Conservation Properties of Least-Squares Finite Element Methods for Scalar Hyperbolic Conservation Laws

29 August 2003

Hans De Sterck

Luke Olson, Tom Manteuffel, Steve McCormick

Department of Applied Mathematics

University of Colorado at Boulder

# Nonlinear hyperbolic conservation law

$$\nabla \cdot \vec{f}(u) = 0 \quad \Omega$$
$$u = g \quad \Gamma_I$$

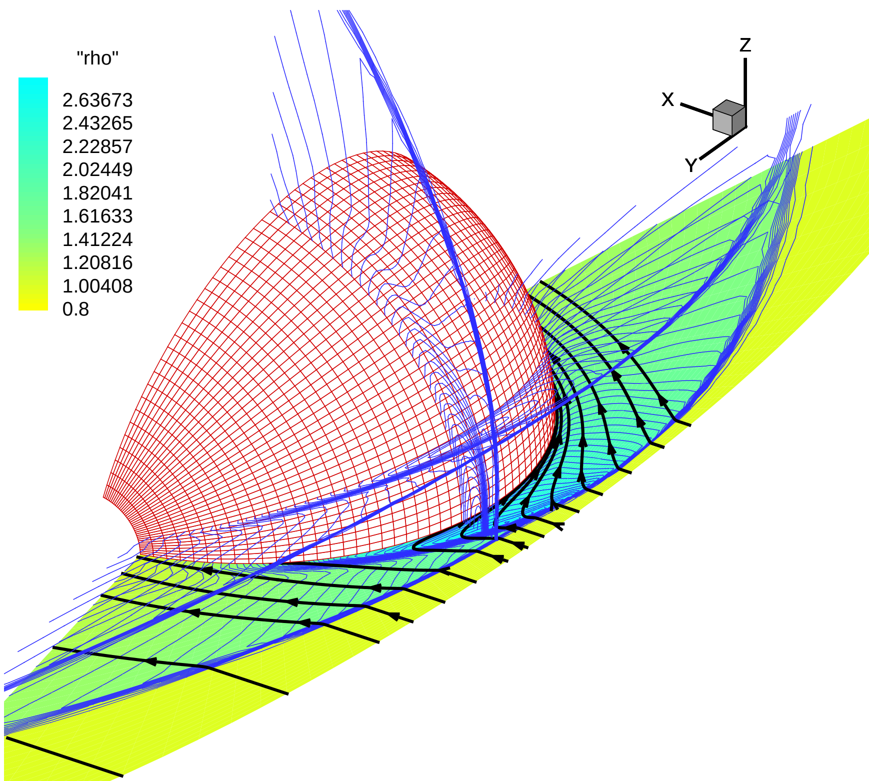
- $u$ scalar
- $\Omega \subset \mathbb{R}^2$ $\qquad$ $\Gamma_I$ inflow boundary
- space-time domains: $\quad \nabla = (\partial_x, \partial_t)$
- example: inviscid Burgers equation:

$$\frac{\partial u^2/2}{\partial x} + \frac{\partial u}{\partial t} = 0 \qquad \text{or} \qquad \vec{f}(u) = (u^2/2, u)$$

- hyperbolic systems: shallow water, Euler, MHD, . . .

# 3D MHD bow shock flows

- PhD thesis research (1999)
- 3D Finite Volume code
- MPI, F90 (64 procs)
- ‘shock-capturing’




- explicit time marching towards steady state
- problems:

(1) small timesteps, many iterations (many 100,000s): need implicit solvers

(2) algorithm not scalable

(3) low order of discretization accuracy (2nd order)

(4) robustness

# This talk: explore alternative approaches

- find approximate solution by minimizing error in a continuous norm
  - – finite difference – finite volume:
    - based on Taylor expansion
      but: not valid for discontinuous solution
    - needs artificial diffusion and nonlinear limiters to make it work anyway (with limitations)
  - – instead: choose norm minimization that is valid for discontinuous solutions – no need for artificial diffusion or limiters
- multi-level linear and nonlinear solvers for scalability

# Some notation

- $L_2$ scalar product

$$\langle f, g \rangle_{0,\Omega} = \int_\Omega f\, g\; dxdt$$

- $L_2$ norm

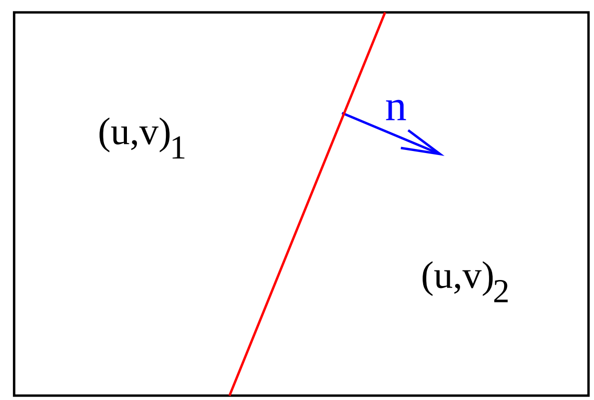
$$\| f \|_{0,\Omega} = \sqrt{\int_\Omega f^2\; dxdt}$$

- space $H(div, \Omega)$

$$\{\ (u, v) \in L_2 \times L_2 \quad | \quad \|\nabla \cdot (u, v)\|^2_{0,\Omega} < \infty\ \}$$

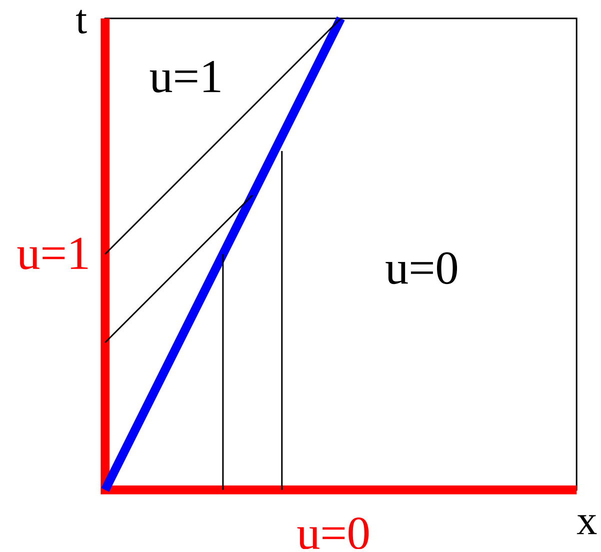
remark: $(u, v)$ can be discontinuous, with normal component continuous

$$\vec{n} \cdot ((u, v)_2 - (u, v)_1) = 0$$



# Weak solutions: discontinuities

$$\nabla \cdot \vec{f}(u) = 0 \quad \Omega$$
$$u = g \quad \Gamma_I$$




- (1) Rankine-Hugoniot relations: $\vec{n} \cdot (\vec{f}(u_2) - \vec{f}(u_1)) = 0$
- (2) equivalent: $\vec{f}(u) \in H(div, \Omega)$
- (3) alternative: $\left\langle \nabla \cdot \vec{f}(u), \phi \right\rangle_{0,\Omega} = 0 \qquad \forall\, \phi \in C^1_{\Gamma_O}(\overline{\Omega})$

or $\quad -\left\langle \vec{f}(u), \nabla\phi \right\rangle_{0,\Omega} + \left\langle \vec{n} \cdot \vec{f}(g), \phi \right\rangle_{0,\Gamma_I} = 0$

$\Rightarrow$ restrict $u$ to piecewise $C^1$ functions with jump discontinuities $\Rightarrow$ *THEOREM:* $\vec{f}(u) \in H(div, \Omega)$

# Outline

- (1) Least-Squares Finite Element Methods
- (2) Standard LSFEM for the Burgers equation
- (3) $H(div)$-conforming LSFEM
- (4) Potential $H(div)$-conforming LSFEM
- (5) Scalable linear solver – AMG
- (6) Scalable nonlinear solver – FMG-Newton
- (7) Numerical conservation – Weak conservation proofs
- Conclusions

# (1) Least-Squares Finite Element Method

- solve $Lu = 0$
- define the functional $\mathcal{F}(u) = \|Lu\|^2_{0,\Omega} = \langle Lu, Lu\rangle_{0,\Omega}$

$\Rightarrow$ minimization: $u^h_* = \underset{u^h \in \mathcal{U}^h}{arg\ min} \|Lu^h\|^2_{0,\Omega} = arg\ min\ \mathcal{F}(u^h)$

- condition for stationary point:

$$\frac{\partial \mathcal{F}(u^h + \alpha v^h)}{\partial \alpha}\Big|_{\alpha=0} = 0 \quad \forall\ v^h \in \mathcal{U}^h$$

if $L$ is linear: $\mathcal{F}(u^h + \alpha v^h) =$

$$\left\langle Lu^h, Lu^h\right\rangle_{0,\Omega} + 2\ \alpha\ \left\langle Lu^h, Lv^h\right\rangle_{0,\Omega} + \alpha^2\ \left\langle v^h, v^h\right\rangle_{0,\Omega}$$

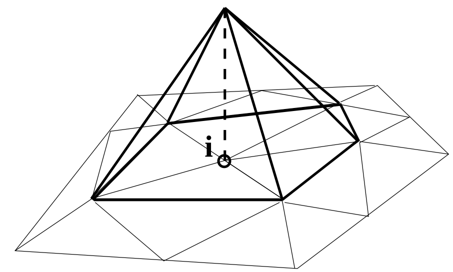
$\Rightarrow$ weak form:

find $u^h \in \mathcal{U}^h$, s.t. $\left\langle Lu^h, Lv^h\right\rangle_{0,\Omega} = 0 \quad \forall v^h \in \mathcal{U}^h$

- btw: LSFEM = FOSLS (First-Order Systems Least-Squares)

# Finite Element Discretization

- approximate $u \in \mathcal{U}$ by $u^h \in \mathcal{U}^h$




$$u^h(t,x) = \sum_{i=1}^{n} u_i\, \phi_i(t,x)$$

- algebraic system from weak form:

$$\left\langle Lu^h, L\phi_j \right\rangle_{0,\Omega} = 0 \qquad \forall \phi_j$$

equation $j$: $\quad \sum_{i=1}^{n} u_i \left\langle L\phi_i, L\phi_j \right\rangle_{0,\Omega} = 0$

(n equations in n unknowns)

# Error Estimator and Adaptive Refinement

$$
\begin{aligned}
\mathcal{F}(u^h) &= \|Lu^h\|_{0,\Omega}^2 \\
&= \|Lu^h - Lu_{exact}\|_{0,\Omega}^2 \\
&= \|L(u^h - u_{exact})\|_{0,\Omega}^2 \\
&= \|Le^h\|_{0,\Omega}^2
\end{aligned}
$$

- functional value gives sharp local a posteriori error estimator
- use error estimator for adaptive refinement in space–time
- error estimator is significant advantage of LSFEM

# (2) LSFEM for the Burgers equation

$$\begin{aligned} \nabla \cdot \vec{f}(u) = 0 & \quad \Omega \\ u = g & \quad \Gamma_I \end{aligned}$$

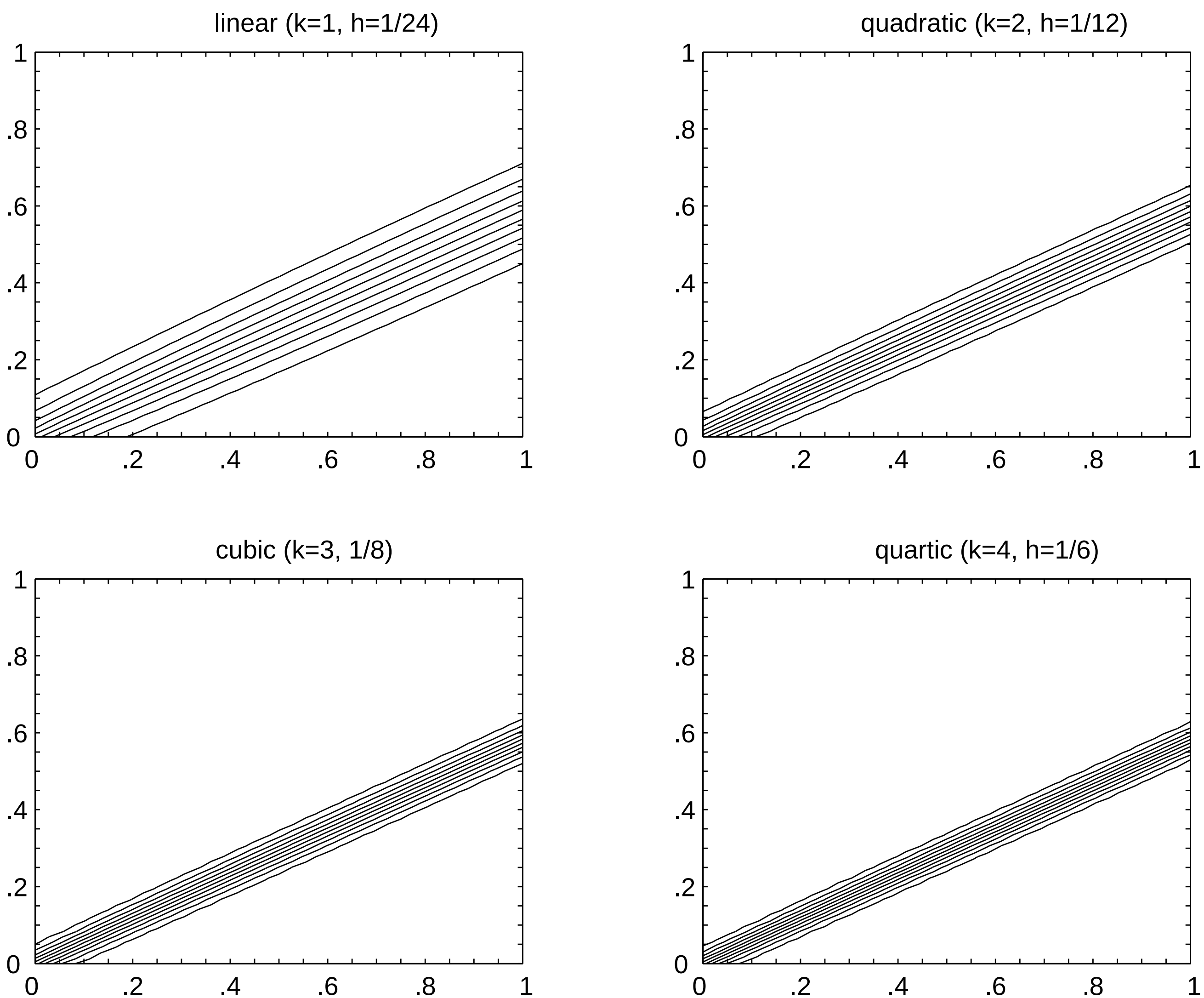
- LS functional

$$\mathcal{H}(u; g) := \|\nabla \cdot \vec{f}(u)\|_{0,\Omega}^2 + \|u - g\|_{0,\Gamma_I}^2$$

- LSFEM

$$u_*^h = \arg\min_{u^h \in \mathcal{U}^h} \mathcal{H}(u^h; g)$$

# Linear advection – higher order schemes



# LSFEM for the Burgers equation

$$\begin{aligned} H(u) := \nabla \cdot \vec{f}(u) = 0 & \quad \Omega \\ u = g & \quad \Gamma_I \end{aligned}$$

- Gauss-Newton minimization of LS functional:
  - first: Newton linearization of $H(u) = 0$

    $$H(u_i) + H'|_{u_i}(u_{i+1} - u_i) = 0$$

    with Fréchet derivative

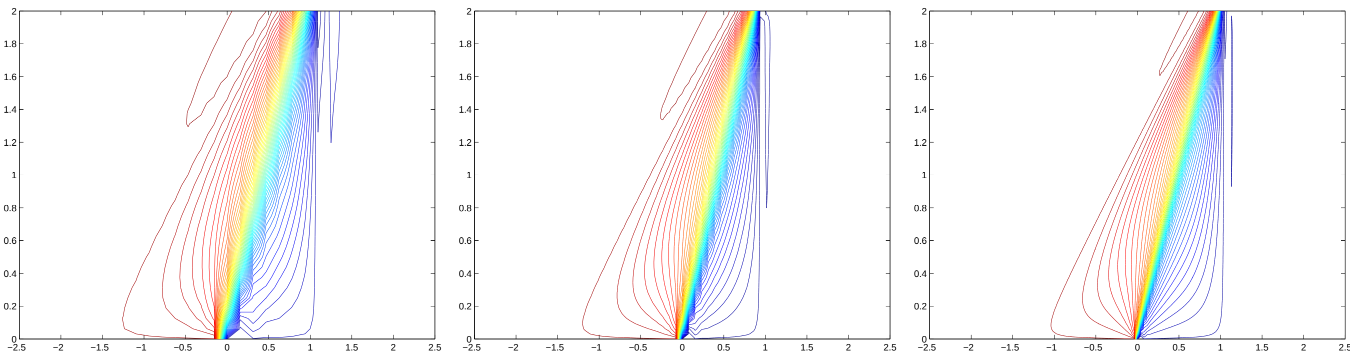
    $$\begin{aligned} H'|_{u_i}(v) &= \lim_{\varepsilon \to 0} \frac{H(u_i + \varepsilon v) - H(u_i)}{\varepsilon} \\ &= \nabla \cdot (\vec{f}'|_{u_i} \, v) \end{aligned}$$

  - then: LS minimization of linearized $H(u)$

    continuous bilinear finite elements on quads for $u^h$

# Numerical Results

shock flow: $u_{left} = 1$, $u_{right} = 0$, shock speed $s = 1/2$



$32^2$ $64^2$ $128^2$

- correct shock speed, no oscillations
- on each grid, Newton process converges
- BUT: for $h \to 0$, nonlinear functional does not go to zero
- this means: for $h \to 0$, convergence to an incorrect solution!!! ($L^*L$ has a spurious stationary point)
- why does LSFEM produce wrong solution??

# Divergence of Newton's method

- reason: Fréchet derivative operator is unbounded

Burgers: $H'|_{u_0}(v) = \nabla \cdot ((u_0, 1)\ v)$

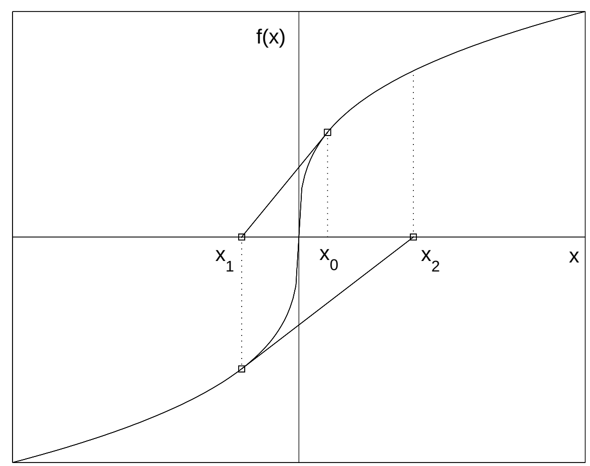
operator $H'|_{u_0}$ :

$$\Rightarrow \|\ H'|_{u_0}\ \|_{0,\Omega} = \infty$$

because for most $v$

$$((u_0, 1)\ v) \notin H(div, \Omega)$$

example: $h(x) = \mp|x|^{1/3}$
$\Rightarrow x_1 = -2x_0$
Newton with $h'(x_*) = \infty$ may have empty basin of attraction



# (3) $H(div)$-conforming LSFEM

- reformulate conservation law in terms of flux vector $\vec{w}$:

$$\begin{aligned} \nabla \cdot \vec{f}(u) &= 0 \quad \Omega \\ u &= g \quad \Gamma_I \end{aligned} \quad \Rightarrow \quad \boxed{\begin{aligned} \nabla \cdot \vec{w} &= 0 & \Omega \\ \vec{w} &= \vec{f}(u) & \Omega \\ \vec{n} \cdot \vec{w} &= \vec{n} \cdot \vec{f}(g) & \Gamma_I \\ u &= g & \Gamma_I \end{aligned}}$$

- Gauss-Newton applied to

$$\begin{aligned} \mathcal{F}(\vec{w}^h, u^h; g) = & \|\nabla \cdot \vec{w}^h\|_{0,\Omega}^2 + \|\vec{w}^h - \vec{f}(u^h)\|_{0,\Omega}^2 \\ & + \|\vec{n} \cdot (\vec{w}^h - \vec{f}(g))\|_{0,\Gamma_I}^2 + \|u^h - g\|_{0,\Gamma_I}^2 \end{aligned}$$

# $H(div)$-conforming LSFEM

- nonlinear operator

$$F(\vec{w},u) := \begin{bmatrix} \nabla\cdot\vec{w} \\ \vec{w}-\vec{f}(u) \end{bmatrix} = 0$$

- Fréchet derivative:

$$F'|_{(\vec{w}_0,u_0)}(\vec{w}_1-\vec{w}_0, u_1-u_0) = \begin{bmatrix} \nabla\cdot & 0 \\ I & -\vec{f}'|_{u_0} \end{bmatrix} \cdot \begin{bmatrix} \vec{w}_1-\vec{w}_0 \\ u_1-u_0 \end{bmatrix}$$

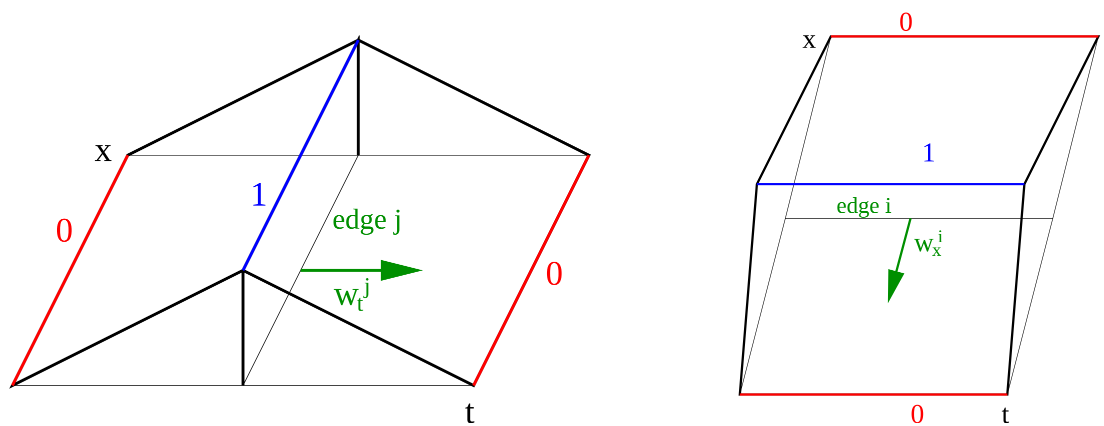
*LEMMA.* Fréchet derivative operator
$F'|_{(\vec{w}_0,u_0)} : H(div,\Omega)\times L^2(\Omega) \longrightarrow L^2(\Omega)$ is bounded:

$$\| \, F'|_{(\vec{w}_0,u_0)} \, \|_{0,\Omega} \le \sqrt{1+K^2}$$

# Finite Element Discretization

- discretize $\vec{w}$ with face elements on quads
  (Raviart-Thomas in 2D): $\vec{w}^h = (w_t^h, w_x^h) \in (V_t^h, V_x^h)$

  face elements: normal vector components are degrees of freedom

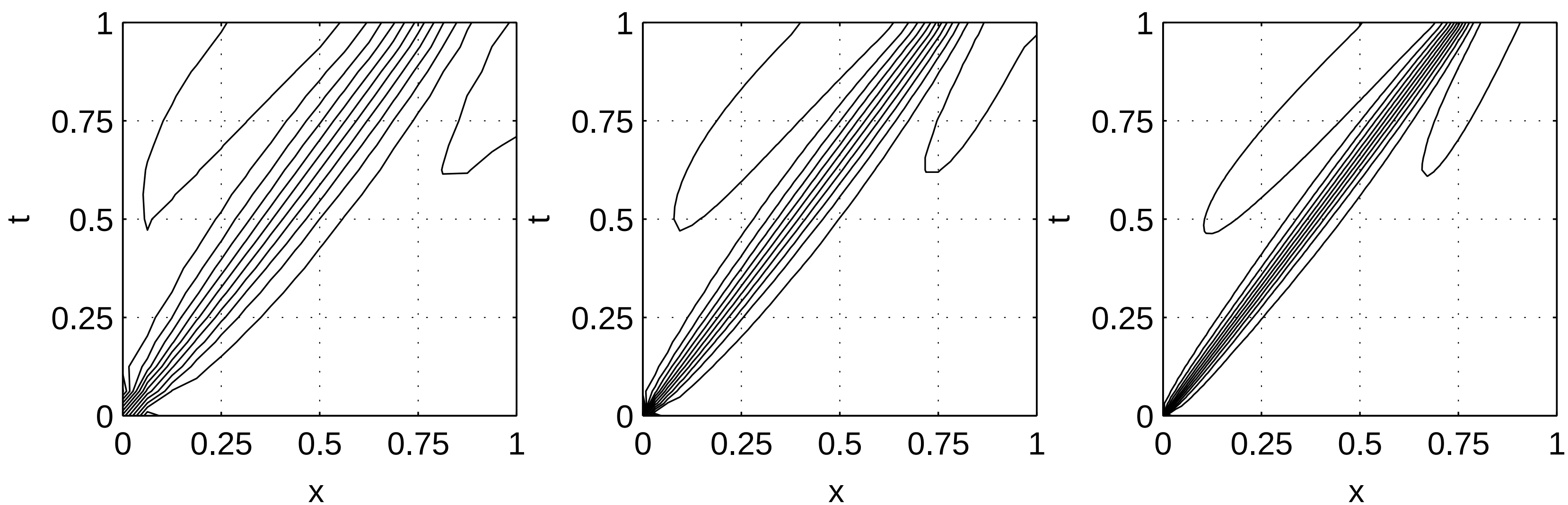



  normal components of $\vec{w}^h$ are continuous
  $\Rightarrow \vec{w}^h \in RT_0 \subset H(div, \Omega)$

- continuous bilinear finite elements on quads for $u^h$

# Numerical results

- shock flow: $u_{left} = 1.0$, $u_{right} = 0.5$, shock speed $s = 0.75$
- $H(div)$-conforming LSFEM:



# Numerical results – convergence study

| $N$ | $\|u^h - u\|^2_{0,\Omega}$ | $\alpha$ | $\mathcal{F}(\vec{w}^h, u^h)$ | $\alpha$ |
|---|---|---|---|---|
| 16 | 5.96e-3 | | 1.89e-2 | |
| | | 0.58 | | 1.03 |
| 32 | 3.81e-3 | | 9.25e-3 | |
| | | 0.69 | | 1.02 |
| 64 | 2.36e-3 | | 4.56e-3 | |
| | | 0.77 | | 1.01 |
| 128 | 1.38e-3 | | 2.26e-3 | |
| | | 0.85 | | 1.01 |
| 256 | 7.66e-4 | | 1.12e-3 | |

# (4) Potential $H(div)$-conforming LSFEM

- define $\nabla^\perp = (-\partial_t, \partial_x)$
- $\nabla \cdot \vec{f}(u) = 0$ implies $\vec{f}(u) = \nabla^\perp \psi$ for some $\psi \in H^1(\Omega)$

$\Rightarrow$ reformulate conservation law in terms of flux potential $\psi$:

$$\begin{aligned} \nabla \cdot \vec{f}(u) &= 0 \quad \Omega \\ u &= g \quad \Gamma_I \end{aligned} \quad \Rightarrow \quad \boxed{\begin{aligned} \nabla^\perp \psi - \vec{f}(u) &= 0 & \Omega \\ \vec{n} \cdot \nabla^\perp \psi &= \vec{n} \cdot \vec{f}(g) & \Gamma_I \\ u &= g & \Gamma_I \end{aligned}}$$

- Gauss-Newton applied to

$$\mathcal{G}(\psi^h, u^h; g) := \\ \|\nabla^\perp \psi^h - \vec{f}(u^h)\|^2_{0,\Omega} + \|\vec{n} \cdot (\nabla^\perp \psi^h - \vec{f}(g))\|^2_{0,\Gamma_I} + \|u^h - g\|^2_{0,\Gamma_I}$$

- $\psi^h$ and $u^h$ continuous bilinear finite elements

# Potential $H(div)$-conforming LSFEM

- nonlinear operator

$$G(\psi, u) := \nabla^{\perp}\psi - \vec{f}(u) = 0$$

- Fréchet derivative:

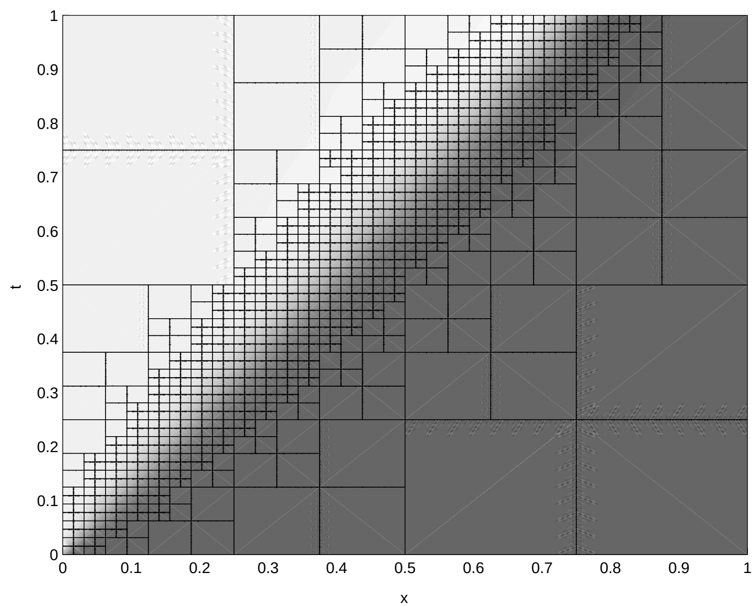
$$G'|_{(\psi_0,u_0)}(\psi_1 - \psi_0, u_1 - u_0) = \left[ \begin{array}{cc} \nabla^{\perp} & -\vec{f'}|_{u_0} \end{array} \right] \cdot \left[ \begin{array}{c} \psi_1 - \psi_0 \\ u_1 - u_0 \end{array} \right]$$

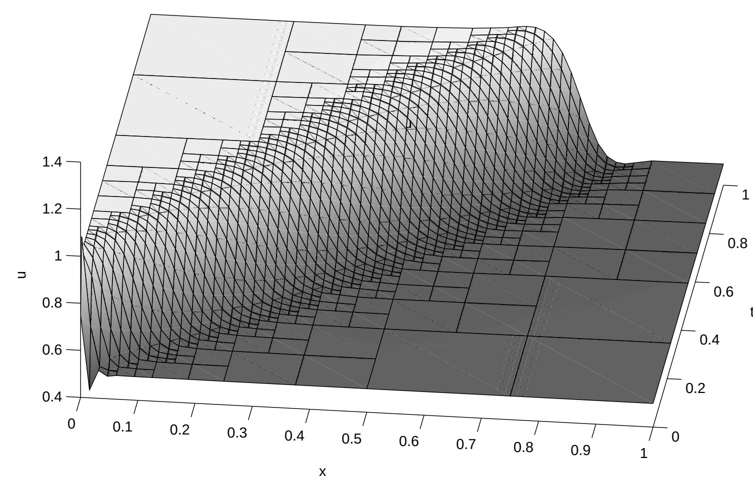
*LEMMA.* Fréchet derivative operator
$G'|_{(\psi_0,u_0)} : H^1(\Omega) \times L^2(\Omega) \to L^2(\Omega)$ is bounded:

$$\| \, G'|_{(\psi_0,u_0)} \, \|_{0,\Omega} \leq \sqrt{1 + K^2}$$

# Numerical results

- potential $H(div)$-conforming LSFEM:




with adaptive refinement in space–time

# (5) Scalable linear solver – AMG

- LSFEM $\Rightarrow$ SPD matrices
- linear hyperbolic PDE
- advection direction $\vec{b} = (\cos\theta, \sin\theta)$

formulation (A)

$$\begin{aligned} \nabla \cdot \vec{b}\, u &= 0 \quad && \Omega \\ u &= g \quad && \Gamma_I \end{aligned}$$

formulation (B)

$$\begin{aligned} \nabla \cdot \vec{b}\, u &= 0 \quad && \Omega \\ u &= g \quad && \Gamma_I \\ \nabla^{\perp}\psi &= \vec{b}\, u \quad && \Omega \\ \nabla^{\perp}\psi &= \vec{b}\, g \quad && \Gamma_I \end{aligned}$$

# Scalable linear solver – boundary conditions

- formulation (A), functional:

$$\|\nabla \cdot \vec{b}\, u^h\|^2_{0,\Omega} + \|u^h - g\|^2_{0,\Gamma_I}$$

matrix equation: $(A_{int} + A_{bndry}) \cdot \vec{x} = \vec{b}$

scale mismatch: $A_{int} = O(1)$, but $A_{bndry} = O(h)$ !

- formulation (B), functional:

$$\|\nabla \cdot \vec{b}\, u^h\|^2_{0,\Omega} + \|u^h - g\|^2_{0,\Gamma_I} + \|\nabla^{\perp}\psi^h - \vec{b}\, u^h\|^2_{0,\Omega} + \|\nabla^{\perp}\psi^h - \vec{b}\, g\|^2_{0,\Gamma_I}$$

right scales: $A_{int} = O(1)$, and also $A_{bndry} = O(1)$ !

$\Rightarrow$ differential boundary condition gives right scale

# AMG interpolation – non-M-matrix

- stencil for $A_{int}$ (formulation (A), $\theta = \pi/4$)

$$\begin{bmatrix} \frac{1}{12} & -\frac{1}{6} & -\frac{5}{12} \\ -\frac{1}{6} & \frac{4}{3} & -\frac{1}{6} \\ -\frac{5}{12} & -\frac{1}{6} & \frac{1}{12} \end{bmatrix}$$

- need special AMG interpolation

# AMG interpolation – non-M-matrix

- interpolate F-point $i$ from surrounding C-points
- guideline

$$A \cdot \vec{e} \approx 0$$

$$-a_{ii}\ e_i = \sum_{j \in C^s} a_{ij}\ e_j + \sum_{j \in C^w} a_{ij}\ e_j + \sum_{j \in F^s} a_{ij}\ e_j + \sum_{j \in F^w} a_{ij}\ e_j$$

| | regular | special |
|---|---|---|
| $C^s$ | keep $e_j$ | keep $e_j$ |
| $C^w$ | to diagonal $e_i$ | to diagonal $e_i$ |
| $F^s$ | to all strong C | to right-sign strong C |
| $F^w$ | to diagonal $e_i$ | to right-sign strong C |

# Scalable linear solver – AMG

- augment equations (formulation (B))
- adjust interpolation, regular V-cycle

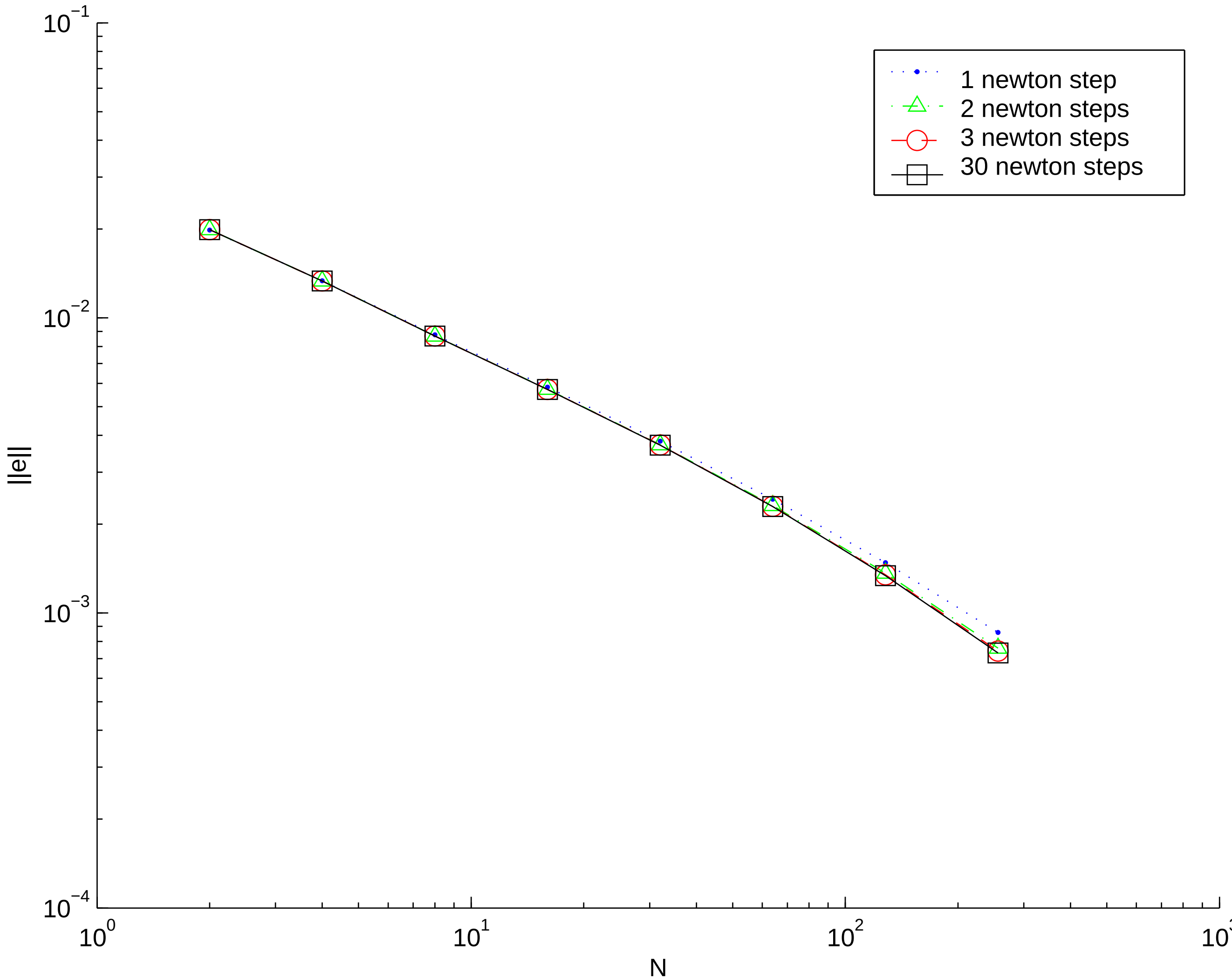
$\Rightarrow$ scalable linear solver

work units (fine-grid relaxation sweeps) per digit of accuracy

$$W_d = \frac{W_c}{-\log \rho_c}$$

| $W_d$ | $128^2$ | $256^2$ | $512^2$ |
|---|---|---|---|
| formulation (A) | 38 | 54 | 79 |
| formulation (B) | 23 | 31 | 31 |

# (6) Scalable nonlinear solver – Newton FMG




$\|u^h - u\|_{0,\Omega}$ convergence: grid continuation (FMG) with only one Newton step per level required!

# (7) Numerical Conservation

nonconservative finite difference schemes can converge to wrong solution!

*THEOREM.* Lax-Wendroff (1960). ‘conservative’ fi nite difference formula:

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0 \quad \rightarrow \quad \frac{u_i^{h,n+1} - u_i^{h,n}}{\Delta t} + \frac{\bar{f}_{i+1/2}^{h,n} - \bar{f}_{i-1/2}^{h,n}}{\Delta x} = 0,$$

exact discrete conservation guarantees convergence to a correct weak solution (assuming convergence of $u^h$ to $\hat{u}$ boundedly a.e.)

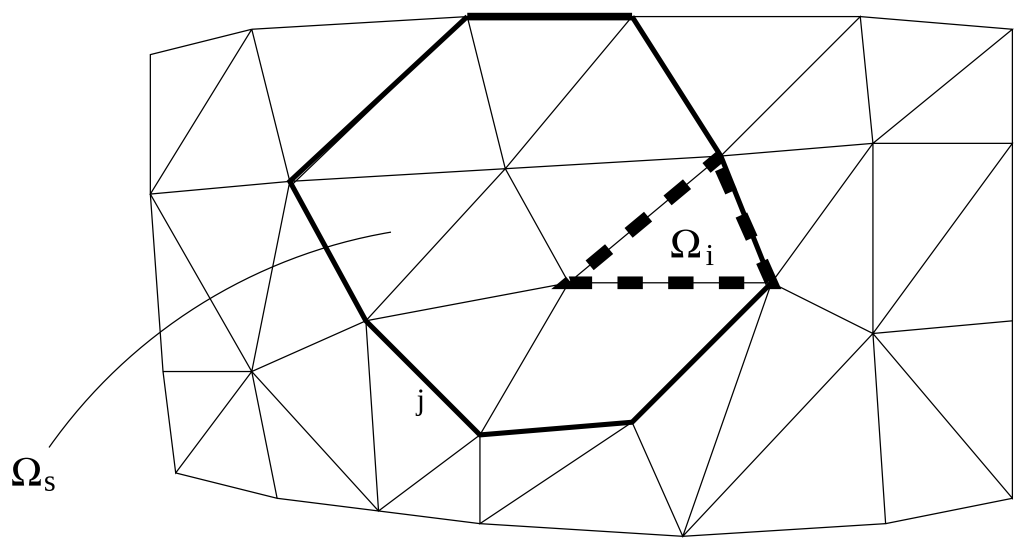
$\Rightarrow$ exact discrete conservation is a *sufficient* condition for convergence to a weak solution

$\Rightarrow$ however, exact discrete conservation is often erroneously considered as a *necessary* condition

# Numerical conservation

- popular FEM for hyperbolic conservation laws (e.g. Discontinuous Galerkin) are discretely conservative in the Lax-Wendroff sense

$$\nabla_{discrete} \cdot \vec{f}(u^h) := \oint_{\partial\Omega_i} \vec{n} \cdot \vec{\bar{f}}(u^h)\, dl = 0 \quad \forall\, \Omega_i$$



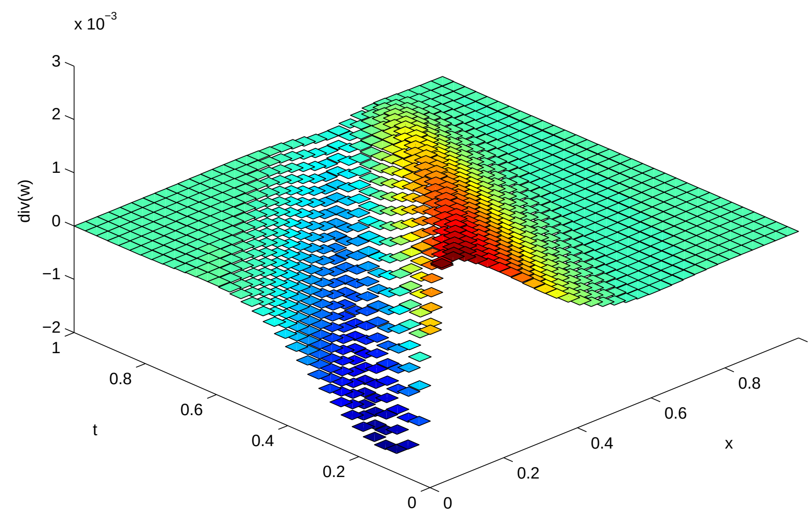
# Numerical conservation

- our $H(div)$-conforming LSFEM do not satisfy the exact discrete conservation property of Lax and Wendroff
- $H(div)$-conforming LSFEM:

$$\nabla \cdot \vec{w} = 0 \qquad \Omega$$

$$\vec{w} = \vec{f}(u) \qquad \Omega$$

$\nabla \cdot \vec{f}(u^h) \neq 0$
(and also $\nabla \cdot \vec{w}^h \neq 0$)




$\nabla \cdot \vec{w}^h$

- potential $H(div)$-conforming LSFEM:

$$\nabla^{\perp}\psi - \vec{f}(u) = 0$$

$\nabla \cdot \vec{f}(u^h) \neq 0$
(but $\nabla \cdot \nabla^{\perp}\psi^h \equiv 0$)

# Numerical conservation

- however, we can prove:

*THEOREM.* [Conservation for $H(div)$-conforming LSFEM]

If finite element approximation $u^h$ converges in the $L^2$ sense to $\hat{u}$ as $h \to 0$, then $\hat{u}$ is a weak solution of the conservation law.

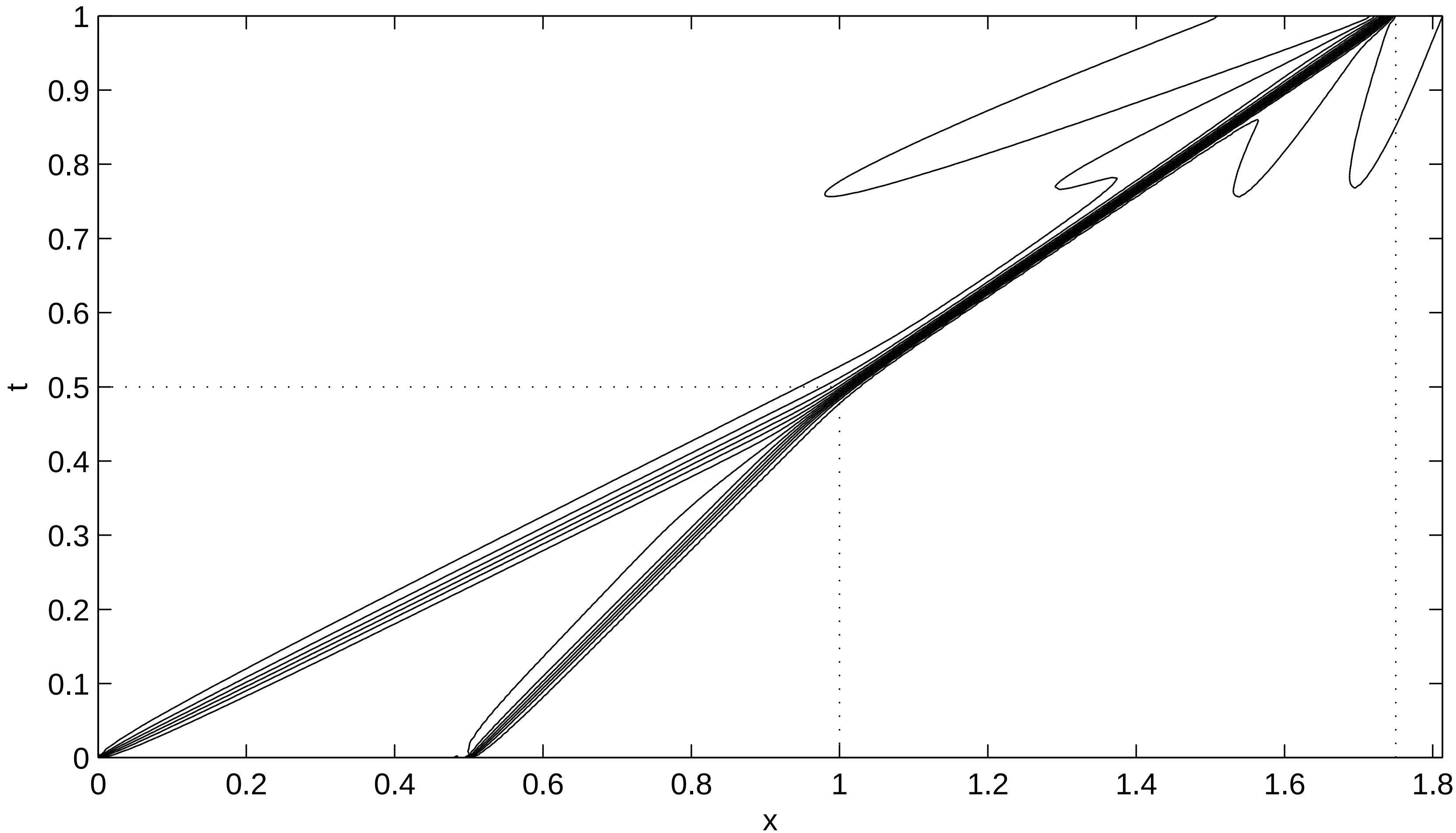
*THEOREM.* [Conservation for potential $H(div)$-conforming LSFEM]

If finite element approximation $u^h$ converges in the $L^2$ sense to $\hat{u}$ as $h \to 0$, then $\hat{u}$ is a weak solution of the conservation law.

$\Rightarrow$ exact discrete conservation is not a necessary condition for numerical conservation!

(can be replaced by minimization in a suitable continuous norm)

# Numerical conservation



# Conclusions

we have developed two classes of $H(div)$-conforming LSFEM for hyperbolic conservation laws

- disadvantages
  - extra variables are introduced ($\vec{w}$ or $\psi$)
  - smearing of LSFEM at shocks, overshoot
- advantages of LSFEM
  - optimal solution within finite element space
  - SPD linear systems (iterative methods, AMG)
  - error estimator (efficient adaptive refinement)
  - non-conservative: convergence to weak solution
  - no spurious oscillations at discontinuities (without need to add numerical diffusion)
  - easy extension to *linear* higher order schemes

# Conclusions

- advantages of flux vector/flux potential reformulations
  - bounded Fréchet derivative $\Rightarrow$ Newton converges
  - smoothness of the solution ($\vec{f}(u) \in H(div, \Omega)$) is made explicit, also at the discrete level using Raviart-Thomas elements ( $\Rightarrow H(div)$-conforming LSFEM)
  - differential part of operator is linear
  - optimal multigrid exists for $H(div)$
- FE convergence theory needs to be worked out further
- scalable AMG results obtained for the potential formulation, parallel scaling being tested (hypre-BoomerAMG)
- methods can be extended to multiple spatial dimensions (using de Rham diagram), and to systems of equations

# Numerical results – convergence study

- estimate $\alpha$ in $\|u^h - u\|^2_{0,\Omega} \approx \mathcal{O}(h^\alpha)$

  $u \in H^{1/2-\epsilon}(\Omega)$ discontinuous $\Rightarrow$ optimal $\alpha = 1.0$

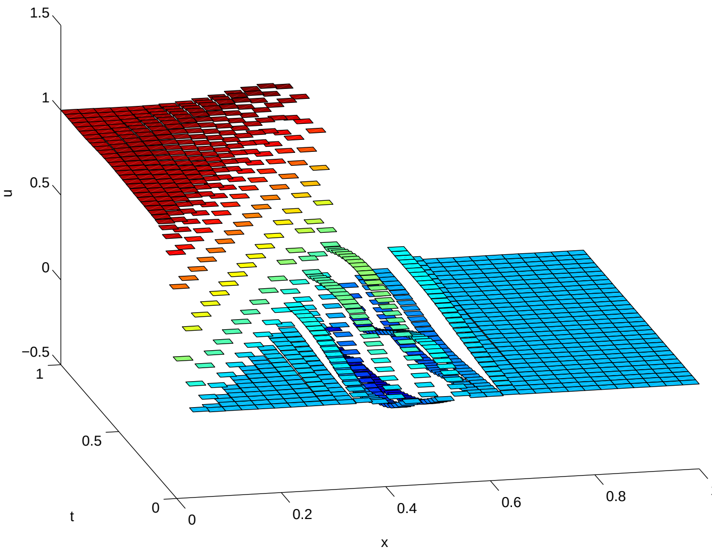
  *i.e.,* $\|u^h - u\|^2_{0,\Omega} \approx \mathcal{O}(h)$, or $\|u^h - u\|_{0,\Omega} \approx \mathcal{O}(h^{1/2})$

- estimate $\alpha$ in $\mathcal{F}(\vec{w}^h, u^h; g) \approx \mathcal{O}(h^\alpha)$

- estimate $\alpha$ in $\mathcal{G}(\psi^h, u^h; g) \approx \mathcal{O}(h^\alpha)$

# Numerical results – choice of spaces

- for $u^h$ piecewise constant (discontinuous): oscillations!




- reason: the functionals are not uniformly coercive
- for right choices of FE spaces (*e.g.*, $u^h$ continuous bilinear), numerical evidence suggests FE convergence
- we have some heuristic understanding of this, but rigorous proofs not yet obtained
- potential formulation is equivalent to $H^{-1}$ minimization

# Hyperbolic PDEs – Conservation Laws

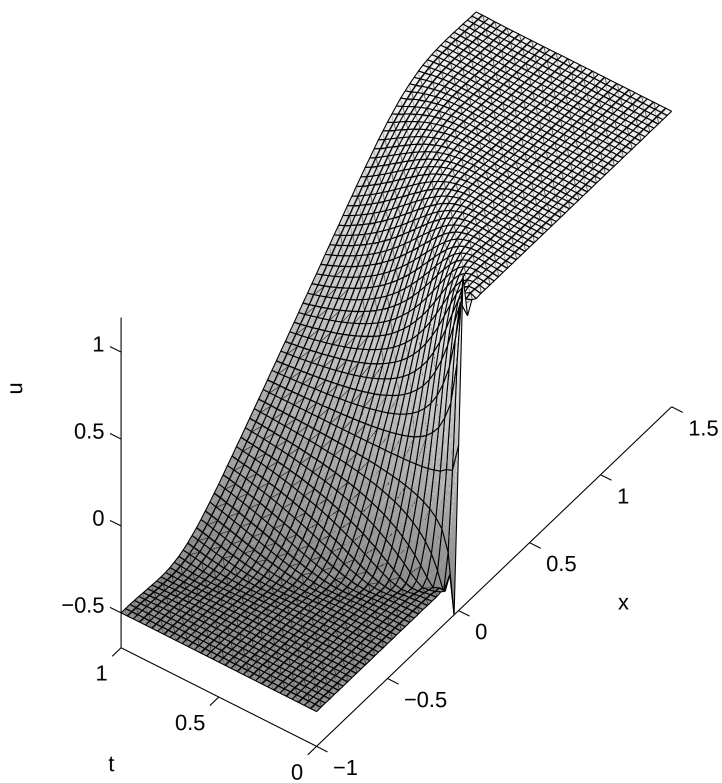
$$\frac{\partial U}{\partial t} + \nabla \cdot \vec{F}(U) = 0$$

- e.g., compressible gases and plasmas
- example: ideal magnetohydrodynamics

$$\frac{\partial}{\partial t}\begin{bmatrix} \rho \\ \rho\vec{v} \\ \rho e \\ \vec{B} \end{bmatrix} + \nabla \cdot \begin{bmatrix} \rho\vec{v} \\ \rho\vec{v}\vec{v} + \left(p + \frac{B^2}{2}\right)\vec{I} - \vec{B}\vec{B} \\ \left(\rho e + p + \frac{B^2}{2}\right)\vec{v} - (\vec{v}\cdot\vec{B})\vec{B} \\ \vec{v}\vec{B} - \vec{B}\vec{v} \end{bmatrix} = 0$$

(fusion plasmas, space plasmas, ...)

# Convergence to entropy solution




- transonic rarefaction
- many weak solutions
- one stable, entropy solution (rarefaction)
- LSFEM converges to entropy solution
- observed in numerical results, no theoretical proof yet