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

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Nonlinear hyperbolic conservation law

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

- u scalar
- $\Omega \subset \mathbb{R}^2$ $\qquad$ Γ_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, ...

This talk: explore alternative approach

- 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

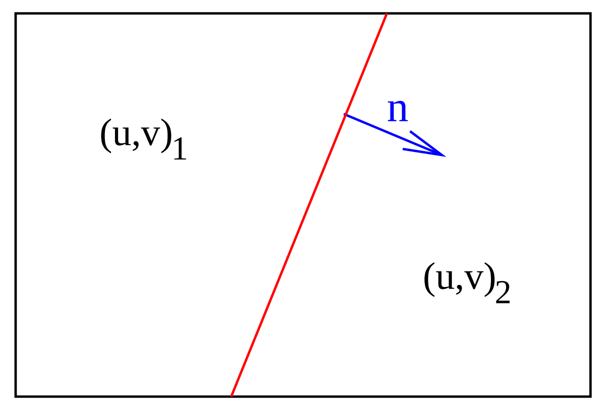
$$\| f \|_{0,\Omega} = \sqrt{\int_\Omega f^2\; dxdt}$$

- space $H(div, \Omega)$

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

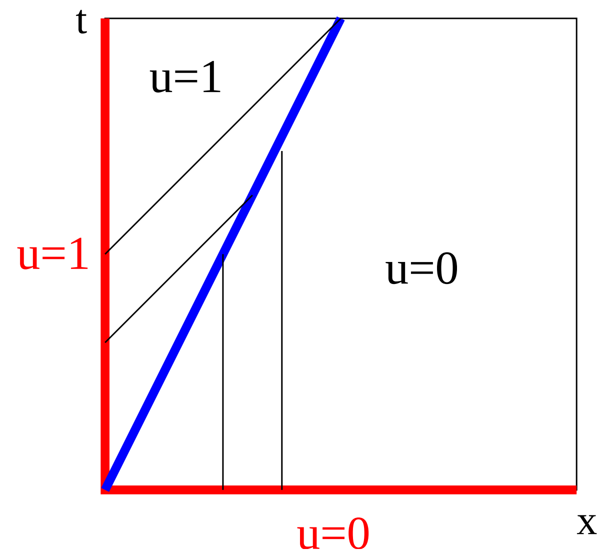
remark: (u,v) can be discontinuous, with normal component continuous

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



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 nonlinear solver – FMG-Newton
- (6) Numerical conservation – Weak conservation proofs

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

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

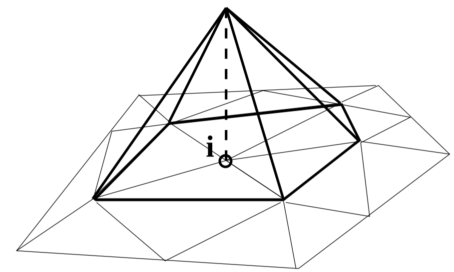
$\Rightarrow$ weak form:

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:

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

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

(n equations in n unknowns)

Error Estimator and Adaptive Refinement

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

- 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

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

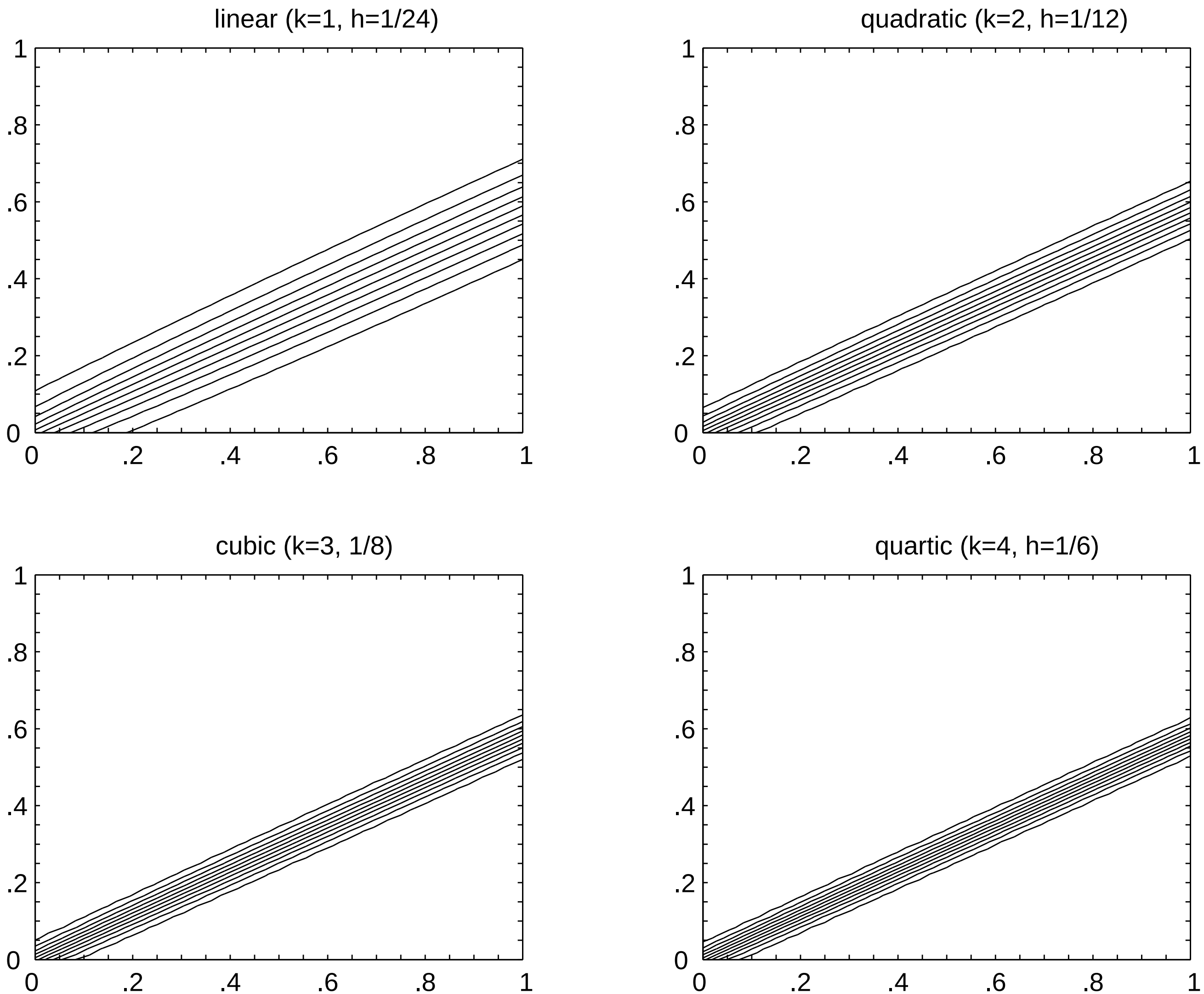
- LS functional

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

- 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

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

- 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

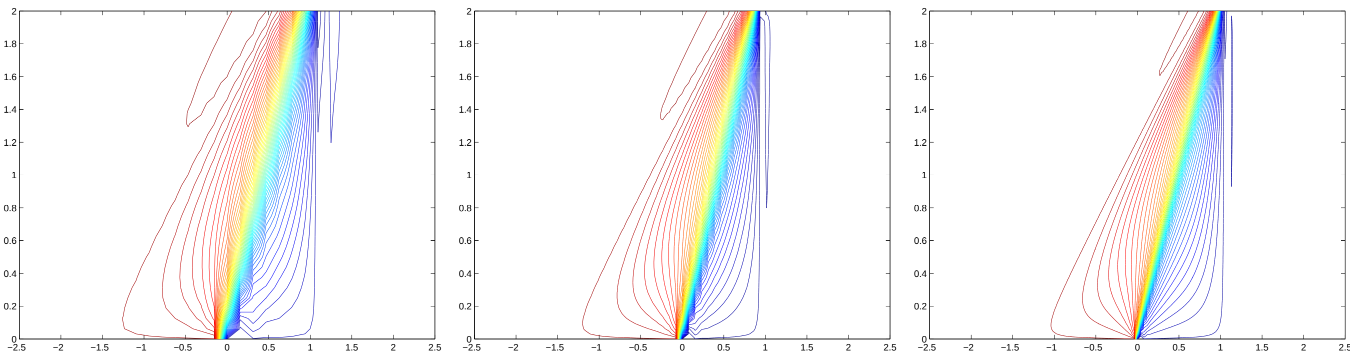
    $$H'|_{u_i}(v) = \lim_{\varepsilon \to 0} \frac{H(u_i + \varepsilon v) - H(u_i)}{\varepsilon} = \nabla \cdot (\vec{f}'|_{u_i}\, v)$$

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

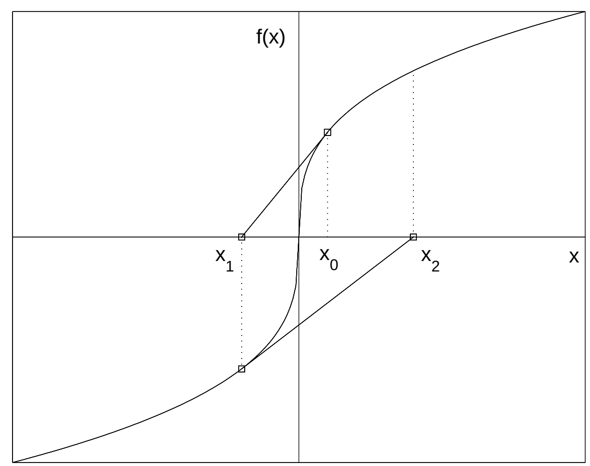
operator $H'|_{u_0}$:

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

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:

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

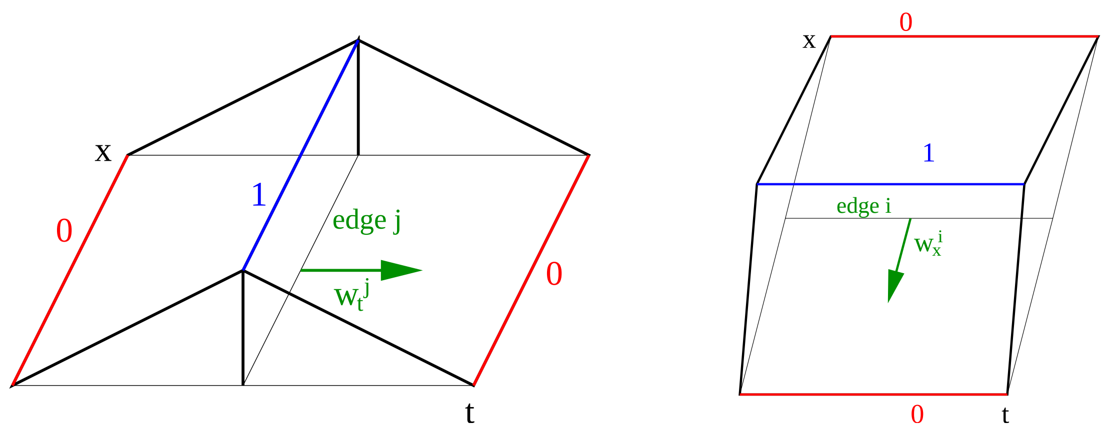
LEMMA. Fréchet derivative operator $F'|_{(\vec{w}_0, u_0)} : H(div, \Omega) \times L^2(\Omega) \to L^2(\Omega)$ is bounded:

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

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

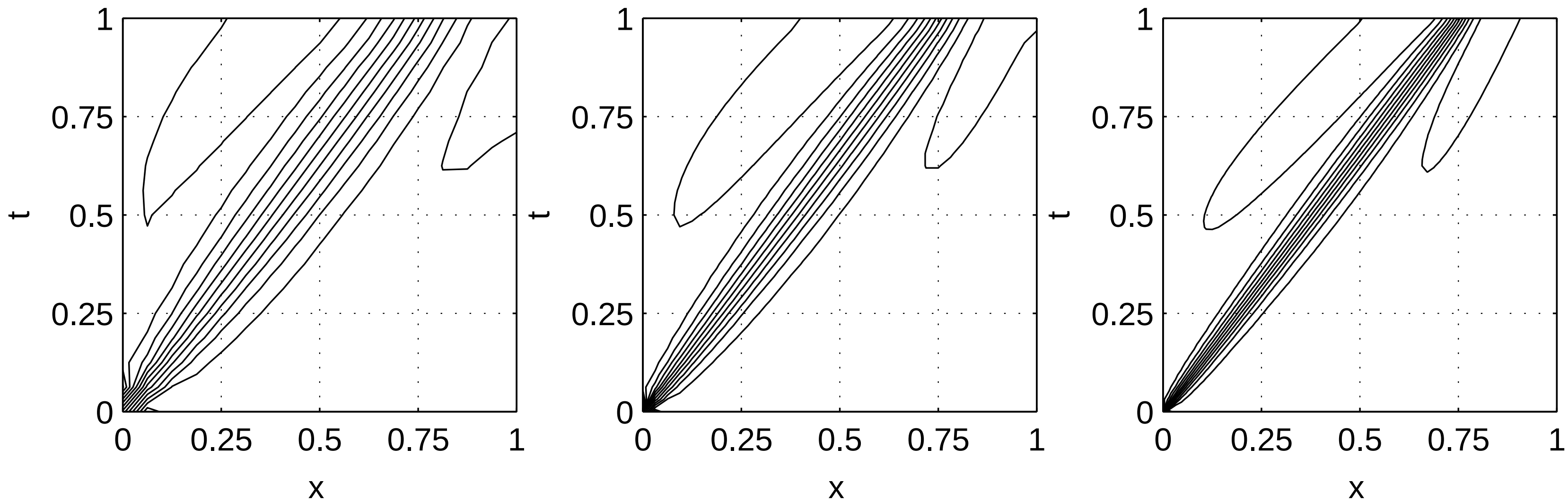


  normal components of $\vec{w}^h$ are continuous
  $\Rightarrow \vec{w}^h \in RT_0 \subset H(div, \Omega)$

- 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	$\|u^h - u\|_{0,\Omega}^2$	α	$\mathcal{F}(\vec{w}^h, u^h)$	α
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 ψ:

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

- Gauss-Newton applied to

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

- ψ^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:

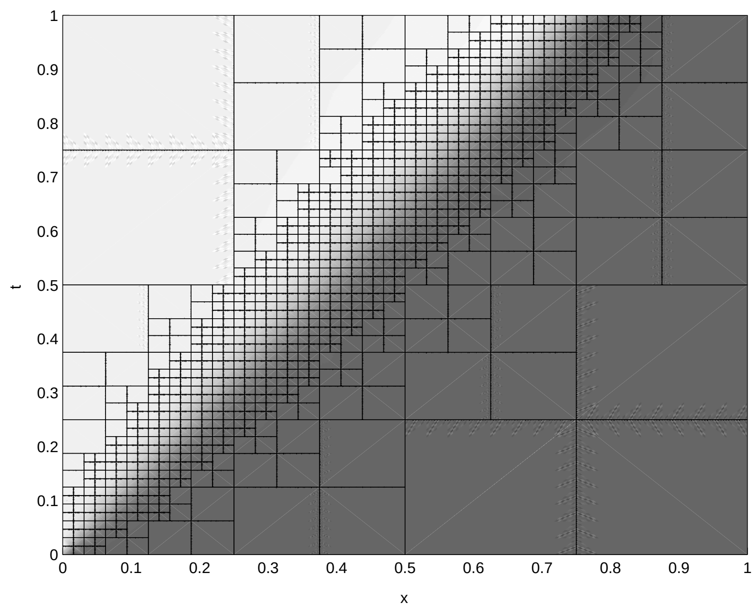
$$G'|_{(\psi_0,u_0)}(\psi_1 - \psi_0, u_1 - u_0) = \begin{bmatrix} \nabla^{\perp} & -\vec{f}'|_{u_0} \end{bmatrix} \cdot \begin{bmatrix} \psi_1 - \psi_0 \\ u_1 - u_0 \end{bmatrix}$$

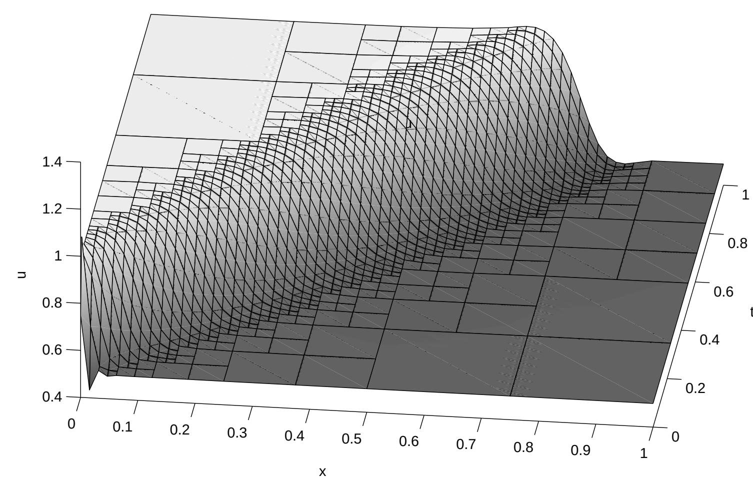
LEMMA. Fréchet derivative operator $G'|_{(\psi_0,u_0)} : H^1(\Omega) \times L^2(\Omega) \to L^2(\Omega)$ is bounded:

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

Numerical results

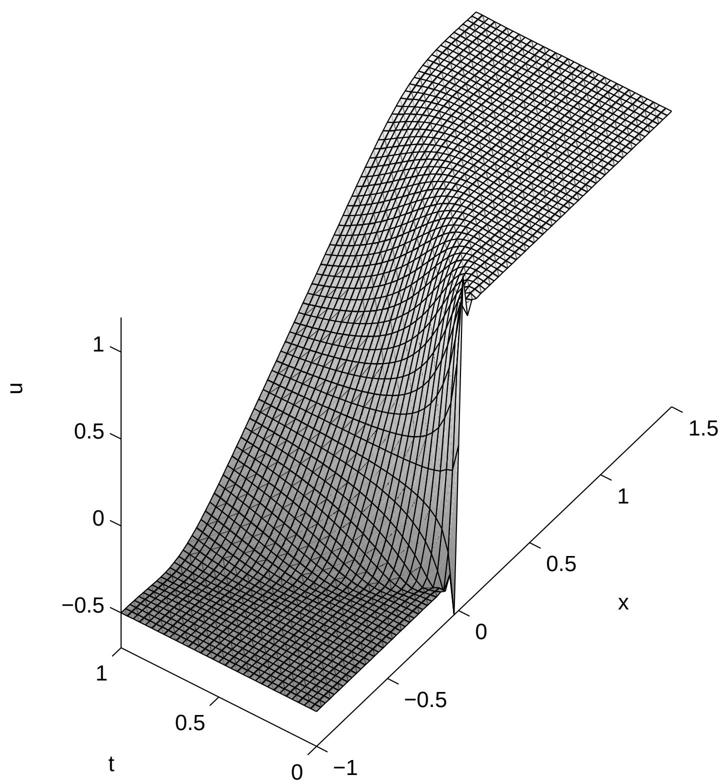
- potential $H(div)$-conforming LSFEM:





with adaptive refinement in space–time

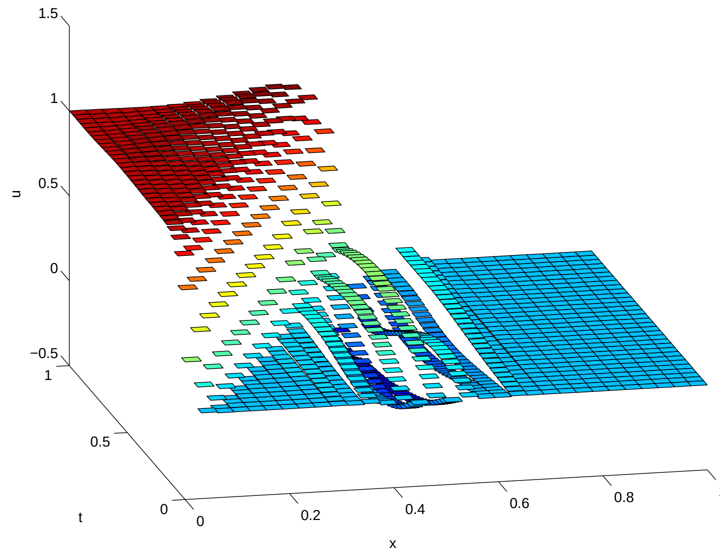
Convergence to entropy solution



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

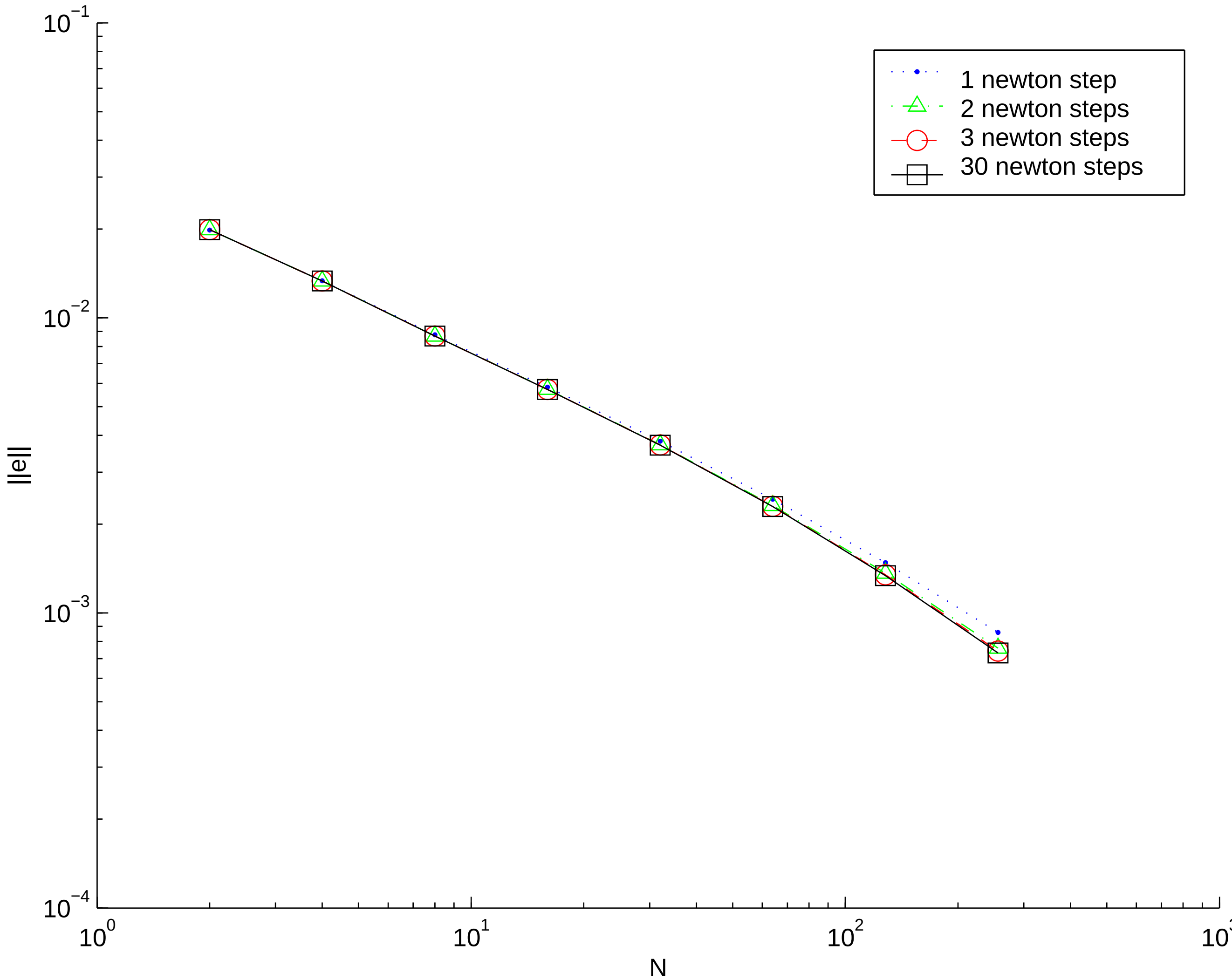
Numerical results – choice of spaces

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



- reason: the functionals are not uniformly coercive w.r.t. L_2 norm
- 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
- weak solution concept problematic?: $H(div)$ not compact in L_2

(5) Scalable nonlinear solver – Newton FMG



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

(6) Numerical Conservation

nonconservative finite difference schemes can converge to wrong solution!

THEOREM. Lax-Wendroff (1960). 'conservative' finite difference formula:

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

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

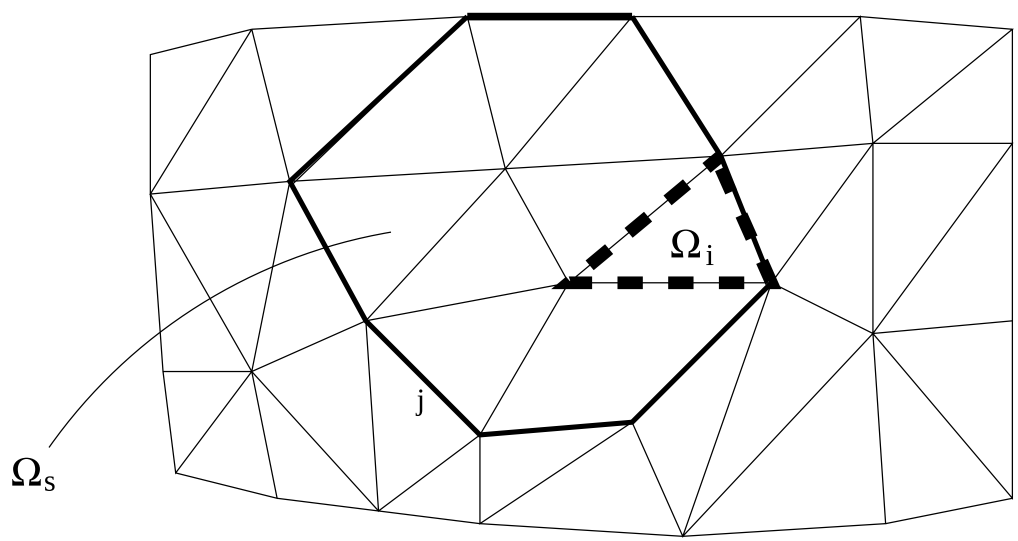
⇒ exact discrete conservation is a *sufficient* condition for convergence to a weak solution

⇒ 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

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



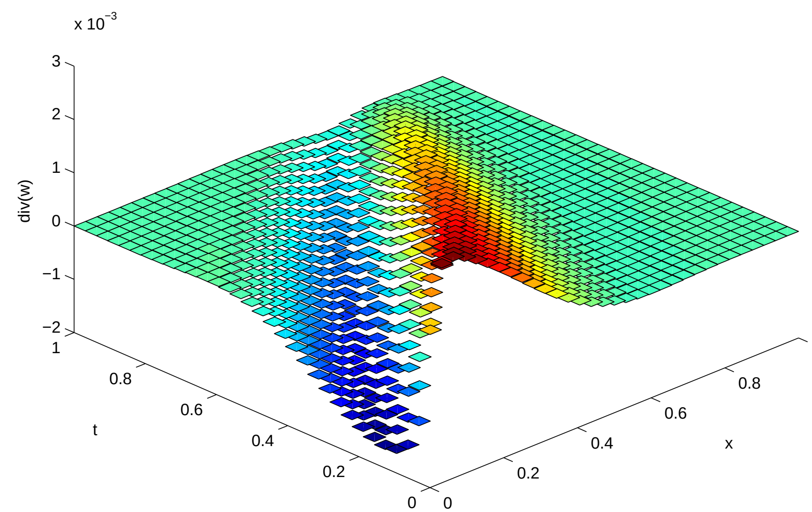
Numerical conservation

- 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 $h \longrightarrow 0$, then $\hat{u}$ is a weak solution of the conservation law.

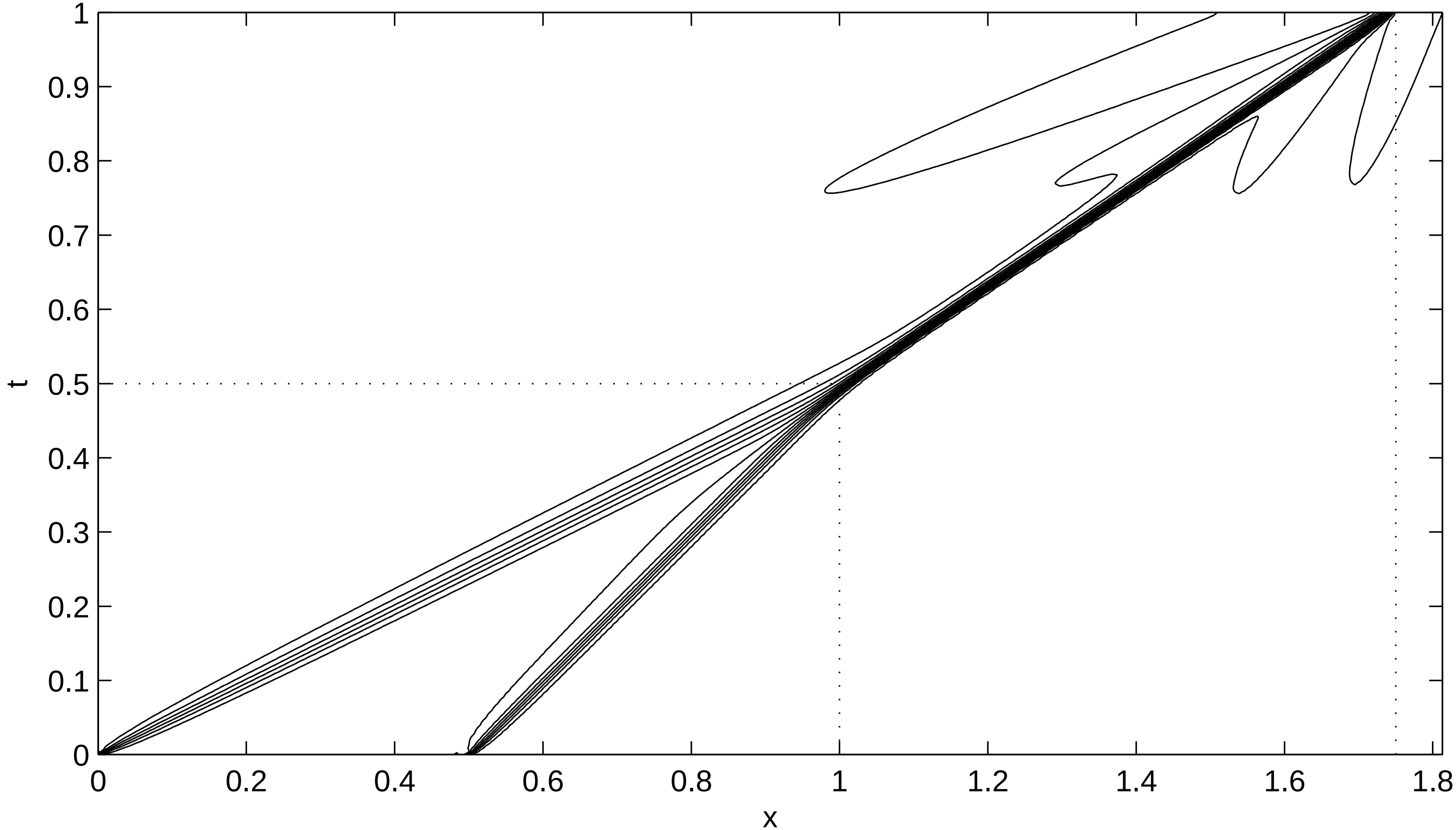
THEOREM. [Conservation for potential $H(div)$-conforming LSFEM]

If finite element approximation u^h converges in the L^2 sense to $\hat{u}$ as $h \longrightarrow 0$, 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 re placed by minimization in a suitable continuous norm)

Numerical conservation



LSFEM for Hyperbolic PDEs: Status

- Burgers equation:
  - nonlinear
  - scalar
  - 2D domains

- extensions, in progress:
  - systems of equations
  - higher-dimensional domains

- need efficient solvers for $A\,u = f$
- need better theoretical understanding

Numerical results – convergence study

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

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

Hyperbolic PDEs – Conservation Laws

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

- 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, . . .)