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Nonlinear hyperbolic conservation law

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

- \( u \) scalar
- \( \Omega \subset \mathbb{R}^2 \quad \Gamma_I \) inflow boundary
- space-time domains: \( \nabla = (\partial_x, \partial_t) \)
- example: inviscid Burgers equation:
  \[ \frac{\partial u^2 / 2}{\partial x} + \frac{\partial u}{\partial t} = 0 \quad \text{or} \quad \vec{f}(u) = (u^2 / 2, u) \]
- 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 $H(div, \Omega)$**
  \[
  \{ \ (u, v) \in L_2 \times L_2 \ | \ \| \nabla \cdot (u, v) \|^2_{0, \Omega} < \infty \ \}
  \]

**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: \( \left< \nabla \cdot \vec{f}(u), \phi \right>_{0, \Omega} = 0 \quad \forall \phi \in C^1_{\Gamma_0}(\Omega) \)

or \( \left< \vec{f}(u), \nabla \phi \right>_{0, \Omega} + \left< \vec{n} \cdot \vec{f}(g), \phi \right>_{0, \Gamma_I} = 0 \)

\[ \Rightarrow \text{restrict } u \text{ to piecewise } C^1 \text{ functions with jump discontinuities} \Rightarrow \quad \text{THEOREM:} \quad \vec{f}(u) \in H(div, \Omega) \]
Outline

• (1) Least-Squares Finite Element Methods
• (2) Standard LSFEM for the Burgers equation
• (3) $H(\text{div})$-conforming LSFEM
• (4) Potential $H(\text{div})$-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 $\mathcal{F}(u) = \|Lu\|_{0,\Omega}^2 = \langle Lu, Lu \rangle_{0,\Omega}$

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

- condition for stationary point:
  $$\frac{\partial \mathcal{F}(u^h + \alpha v^h)}{\partial \alpha} \bigg|_{\alpha=0} = 0 \quad \forall v^h \in \mathcal{U}^h$$

  if $L$ is linear: $\mathcal{F}(u^h + \alpha v^h) =
  \langle Lu^h, Lu^h \rangle_{0,\Omega} + 2 \alpha \langle Lu^h, Lv^h \rangle_{0,\Omega} + \alpha^2 \langle v^h, v^h \rangle_{0,\Omega}$

$\Rightarrow$ weak form:

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

- 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:

\[
\langle Lu^h, L\phi_j \rangle_{0, \Omega} = 0 \quad \forall \phi_j
\]

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

\[ F(u^h) = \| Lu^h \|_{0,\Omega}^2 \]
\[ = \| Lu^h - Lu_{exact} \|_{0,\Omega}^2 \]
\[ = \| L(u^h - u_{exact}) \|_{0,\Omega}^2 \]
\[ = \| L e^h \|_{0,\Omega}^2 \]

- 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

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

- 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

Linear (k=1, h=1/24)

Quadratic (k=2, h=1/12)

Cubic (k=3, 1/8)

Quartic (k=4, h=1/6)
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 \( s = 1/2 \)

- 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: \[ H'\mid_{u_0}(v) = \nabla \cdot ((u_0, 1) \cdot v) \]

operator \( H'\mid_{u_0} \):

\[ \Rightarrow \| H'\mid_{u_0} \|_{0, \Omega} = \infty \]

because for most \( v \)

\[ ((u_0, 1) \cdot v) \notin H(div, \Omega) \]

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 $\vec{w}$:

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

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

- Gauss-Newton applied to

\[
\mathcal{F}(\vec{w}^h, u^h; g) = \|\nabla \cdot \vec{w}^h\|_{0,\Omega}^2 + \|\vec{w}^h - \vec{f}(u^h)\|_{0,\Omega}^2 \\
+ \|\vec{n} \cdot (\vec{w}^h - \vec{f}(g))\|_{0,\Gamma_I}^2 + \|u^h - g\|_{0,\Gamma_I}^2
\]
$H(div)$-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): $\vec{w}^h = (w^h_t, w^h_x) \in (V^h_t, V^h_x)$

  face elements: normal vector components are degrees of freedom

  \[ \vec{w}^h_{RT0} \subseteq H(div, \Omega) \]

- 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:**

![Graphs illustrating numerical results](image-url)
## Numerical results – convergence study

<table>
<thead>
<tr>
<th>$N$</th>
<th>$|u^h - u|_{0,\Omega}^2$</th>
<th>$\alpha$</th>
<th>$F(\overline{w}^h, u^h)$</th>
<th>$\alpha$</th>
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<td>256</td>
<td>7.66e-4</td>
<td></td>
<td>1.12e-3</td>
<td></td>
</tr>
</tbody>
</table>
(4) Potential \( H(\text{div}) \)-conforming LSFEM

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

\[ \Rightarrow \text{reformulate conservation law in terms of flux potential } \psi: \]

\[
\begin{align*}
\nabla \cdot \vec{f}(u) &= 0 \quad \Omega \\
u &= g \quad \Gamma_I
\end{align*}
\]

\[ \Rightarrow \begin{cases} 
\nabla^\perp \psi - \vec{f}(u) = 0 & \Omega \\
\vec{n} \cdot \nabla^\perp \psi = \vec{n} \cdot \vec{f}(g) & \Gamma_I \\
u &= g & \Gamma_I
\end{cases} \]

- Gauss-Newton applied to

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

- \( \psi^h \) and \( u^h \) continuous bilinear finite elements
Potential $H^{(\text{div})}$-conforming LSFEM

- nonlinear operator
  \[ G(\psi, u) := \nabla^\perp \psi - \tilde{f}(u) = 0 \]

- Fréchet derivative:
  \[ G''|_{(\psi_0, u_0)}(\psi_1 - \psi_0, u_1 - u_0) = \begin{bmatrix} \nabla^\perp & -\tilde{f}'|u_0 \end{bmatrix} \cdot \begin{bmatrix} \psi_1 - \psi_0 \\ u_1 - u_0 \end{bmatrix} \]

**Lemma.** Fréchet derivative operator
\[ G''|_{(\psi_0, u_0)} : H^1(\Omega) \times L^2(\Omega) \rightarrow L^2(\Omega) \] 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:

\[
\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0 \quad \Rightarrow \quad \frac{u_{i}^{h,n+1} - u_{i}^{h,n}}{\Delta t} + \frac{f_{i+1/2}^{h,n} - f_{i-1/2}^{h,n}}{\Delta x} = 0,
\]

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

\[ \nabla_{\text{discrete}} \cdot \vec{f}(u^h) := \oint_{\partial \Omega_i} \vec{n} \cdot \vec{f}(u^h) \, dl = 0 \quad \forall \, \Omega_i \]
Numerical conservation

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

- $H(\text{div})$-conforming LSFEM:

\[
\nabla \cdot \vec{w} = 0 \quad \Omega \\
\vec{w} = \vec{f}(u) \quad \Omega \\
\nabla \cdot \vec{f}(u^h) \neq 0 \\
\text{(and also } \nabla \cdot \vec{w}^h \neq 0) \\
\]

- potential $H(\text{div})$-conforming LSFEM:

\[
\nabla^\perp \psi - \vec{f}(u) = 0 \\
\nabla \cdot \vec{f}(u^h) \neq 0 \\
\text{(but } \nabla \cdot \nabla^\perp \psi^h \equiv 0) 
\]
Numerical conservation

- however, we can prove:

**THEOREM.** [Conservation for \( H(\text{div}) \)-conforming LSFEM]

If finite element approximation \( \mathcal{d}_h \) converges in the \( L^2 \) sense to \( \mathcal{d} \) as \( h \to 0 \), then \( \mathcal{d} \) is a weak solution of the conservation law.

**THEOREM.** [Conservation for potential \( H(\text{div}) \)-conforming LSFEM]

If finite element approximation \( \mathcal{d}_h \) converges in the \( L^2 \) sense to \( \mathcal{d} \) as \( h \to 0 \), then \( \mathcal{d} \) 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
LSFEM for Hyperbolic PDEs: Status

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

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

- need efficient solvers for $Au = f$
- need better theoretical understanding
Numerical results – convergence study

- estimate $\alpha$ in $\|u^h - u\|_{0,\Omega}^2 \approx \mathcal{O}(h^\alpha)$
  
  $u \in H^{1/2-\epsilon}(\Omega)$ discontinuous $\Rightarrow$ optimal $\alpha = 1.0$
  
  i.e., $\|u^h - u\|_{0,\Omega}^2 \approx \mathcal{O}(h)$, or $\|u^h - u\|_{0,\Omega} \approx \mathcal{O}(h^{1/2})$

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

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

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

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

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

(fusion plasmas, space plasmas, . . . )