 Least-Squares Finite Element Methods for Nonlinear Hyperbolic PDEs

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Outline

(1) Hyperbolic Conservation Laws: Introduction

(2) Least-Squares Finite Element Methods

(3) Fluid Dynamics Applications
(1) Numerical Simulation of Nonlinear Hyperbolic PDE Systems

Example application: gas dynamics

- supersonic flow of air over sphere (M=1.53)
- bow shock
- (An album of fluid motion, Van Dyke)
Nonlinear Hyperbolic Conservation Laws

- Euler equations of gas dynamics

\[
\frac{\partial}{\partial t} \begin{bmatrix}
\rho \\
\rho \vec{v} \\
\rho e
\end{bmatrix} + \nabla \cdot \begin{bmatrix}
\rho \vec{v} \\
\rho \vec{v} \vec{v} + p \vec{I} \\
(\rho e + p(\rho, e)) \vec{v}
\end{bmatrix} = 0
\]

- Nonlinear hyperbolic PDE system

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

- Conservation law

\[
\frac{\partial}{\partial t} \left( \int_{\Omega} U \, dV \right) + \int_{\partial\Omega} \vec{n} \cdot \vec{F}(U) \, dA = 0
\]
Model Problem: Scalar Inviscid Burgers Equation

- scalar conservation law in 1D

\[ \frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0 \]

- model problem: inviscid Burgers equation

\[ \frac{\partial u}{\partial t} + \frac{\partial u^2/2}{\partial x} = 0 \]
Burgers Equation: Model Flow

\[ \frac{\partial u}{\partial t} + \frac{u^2}{2} \frac{\partial}{\partial x} = 0 \]

- hyperbolic PDE: information propagates along characteristic curves
- \( u \) is constant on characteristic
- \( u \) is slope of characteristic
- where characteristics cross:
  - shock formation (weak solution)
Space-Time Formulation

\[ \frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0 \]

- define \( \nabla_{x,t} = (\partial_x, \partial_t) \)
- define \( \vec{f}_{x,t}(u) = (f(u), u) \)

\[ \nabla_{x,t} \cdot \vec{f}_{x,t}(u) = 0 \quad \Omega \subset \mathbb{R}^2 \]
\[ u = g \quad \Gamma_I \]

- conservation in space-time

\[ \oint_{\Gamma} \vec{n}_{x,t} \cdot \vec{f}_{x,t}(u) \, dl = 0 \]
Some Notation

- \( L_2 \) scalar product
  \[
  \langle f, g \rangle_{0,\Omega} = \int_{\Omega} f g \, dx dt
  \]

- \( L_2 \) norm
  \[
  \| f \|_{0,\Omega} = \sqrt{\int_{\Omega} f^2 \, dx dt}
  \]

- space \( H(\text{div}, \Omega) \)
  \[
  \{ (u, v) \in L_2 \times L_2 \mid \| \nabla \cdot (u, v) \|_{0,\Omega}^2 < \infty \}
  \]

remark: \((u, v)\) can be discontinuous, with normal component continuous:
\[
\bar{n} \cdot ((u, v)_2 - (u, v)_1) = 0
\]
Weak Solutions: Discontinuities

\[ \nabla_{x,t} \cdot \vec{f}_{x,t}(u) = 0 \quad \Omega \]

\[ u = g \quad \Gamma_I \]

(1) Rankine-Hugoniot relations:

\[ \vec{n}_{x,t} \cdot (\vec{f}_{x,t}(u_2) - \vec{f}_{x,t}(u_1)) = 0 \]

(2) equivalent:

\[ \vec{f}_{x,t}(u) \in H(div, \Omega) \quad \text{(solution regularity)} \]

Burgers model flow:

\[ \vec{f}_{x,t}(u) \in H(div, \Omega) \iff \text{shock speed} \ s = \frac{1}{2} \]
Numerical Approximation: Finite Differences

- derivatives \( \Rightarrow \) use truncated Taylor series expansion

\[
\frac{\partial u}{\partial x}\bigg|_i = \frac{u_i - u_{i-1}}{\Delta x} + O(\Delta x)
\]

- Burgers:

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0 \Rightarrow \frac{u_{i,n+1}^h - u_{i,n}^h}{\Delta t} + u_{i,n}^h \frac{u_{i,n}^h - u_{i-1,n}^h}{\Delta x} = 0
\]

\( \Rightarrow \) convergence to wrong solution!

- reason: Taylor expansion not valid at shock!
**Conservative Finite Difference Schemes**

**THEOREM.** Lax-Wendroff (1960).

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

**Theorem:** conservative finite difference scheme guarantees convergence to a correct weak solution (assuming convergence of \(u^h\) to some \(\hat{u}\))

\[\Rightarrow \text{‘conservative’ form is a } \text{**sufficient**} \text{ condition for convergence to a weak solution (but it may not be } \text{**necessary**}! \ldots \)\]
Why the Name ‘Conservative Scheme’?

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

\[ \oint_{\partial \Omega_i} \vec{n}_{x,t} \cdot (\bar{f}(u^h), u^h) \, dl = 0 \quad \forall \, \Omega_i \]

- recall conservation in space-time
  \[ \oint_{\partial \Omega} \vec{n}_{x,t} \cdot \bar{f}_{x,t}(u) \, dl = 0 \]

⇒ exact discrete conservation in every discrete cell \( \Omega_i \)

- exact discrete conservation constrains the solution, s.t. convergence to a solution with wrong shock speed cannot happen
Lax-Wendroff Scheme

\[
\tilde{f}_{i+1/2} = \frac{1}{2} \left( \left( \frac{u_{i+1}}{2} \right)^2 + \left( \frac{u_i}{2} \right)^2 - \frac{\Delta t}{\Delta x} \left( \frac{u_i + u_{i+1}}{2} \right)^2 (u_{i+1} - u_i) \right)
\]

- conservative
- \(O(\Delta x^2)\) (Taylor)
- correct shock speed
- \ldots oscillations!
Possible Remedy: Numerical Diffusion

- add numerical diffusion

\[ \frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = \eta_{num} \frac{\partial^2 u}{\partial x^2} \]

- \( \eta_{num} = O(\Delta x^2) \), e.g.
- problem: need nonlinear limiters
- problem: higher-order difficult

- this ‘stabilization by numerical diffusion’ approach is employed in
  - upwind schemes
  - finite volume schemes
  - most existing finite element schemes
Alternative: Solution Control through Functional Minimization

- minimize the error in a continuous norm

\[ u^h_* = \arg \min_{u^h \in U^h} \| \nabla x, t \cdot \tilde{f}_x, t (u^h) \|_{0, \Omega}^2 \]

- goal:
  - control oscillations
  - control convergence to weak solution
  - control numerical stability (no need for time step limitation)
  - higher-order finite elements

⇒ achieve through norm minimization

(remark: \( h = \Delta x \))
(2) Least-Squares Finite Element (LSFEM) Discretizations

with Luke Olson, Tom Manteuffel, Steve McCormick, Applied Math CU Boulder

- finite element method: approximate $u \in \mathcal{U}$ by $u^h \in \mathcal{U}^h$

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

- abstract example: solve $Lu = 0$ (assume $L$ linear PDE operator)

- define the functional $\mathcal{F}(u) = \|Lu\|_{0,\Omega}^2$
Least-Squares Finite Element (LSFEM) Discretizations

⇒ minimization:

\[ u^h = \arg \min_{u^h \in \mathcal{U}^h} \| Lu^h \|^2_{0, \Omega} = \arg \min \mathcal{F}(u^h) \]

• condition for \( u^h \) stationary point:

\[ \left. \frac{\partial \mathcal{F}(u^h + \alpha v^h)}{\partial \alpha} \right|_{\alpha=0} = 0 \quad \forall v^h \in \mathcal{U}^h \]
Least-Squares Finite Element Discretizations

- algebraic system of linear equations:

\[ \sum_{i=1}^{n} u_i \langle L\phi_i, L\phi_j \rangle_{0,\Omega} = 0 \]

(n equations in n unknowns, \( A u = 0 \))

(actually, with boundary conditions, \( A u = f \))

- Symmetric Positive Definite (SPD) matrices \( A \)
$H(div)$-Conforming LSFEM for Hyperbolic Conservation Laws

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

$$\nabla_{x,t} \cdot \vec{f}_{x,t}(u) = 0 \quad \Omega$$
$$u = g \quad \Gamma_I$$

$$\Rightarrow$$

$$\nabla_{x,t} \cdot \vec{w} = 0 \quad \Omega$$
$$\vec{w} = \vec{f}_{x,t}(u) \quad \Omega$$
$$\vec{n}_{x,t} \cdot \vec{w} = \vec{n}_{x,t} \cdot \vec{f}_{x,t}(g) \quad \Gamma_I$$
$$u = g \quad \Gamma_I$$

- Functional

$$\mathcal{F}(\vec{w}^h, u^h; g) = \| \nabla_{x,t} \cdot \vec{w}^h \|_{0,\Omega}^2 + \| \vec{w}^h - \vec{f}^h(u^h) \|_{0,\Omega}^2$$
$$+ \| \vec{n}_{x,t} \cdot (\vec{w}^h - \vec{f}^h(g)) \|_{0,\Gamma_I}^2 + \| u^h - g \|_{0,\Gamma_I}^2$$

- Newton linearization: minimize functional with linearized equation
Finite Element Spaces

- weak solution: \( \tilde{f}_{x,t} \in H(\text{div}, \Omega) \)
  \( \Rightarrow \) choose \( \tilde{w}^h \in H(\text{div}, \Omega) \)

- Raviart-Thomas elements: the normal components of \( \tilde{w}^h \) are continuous
  \( \Rightarrow \tilde{w}^h \in H(\text{div}, \Omega) \)

\( \Rightarrow H(\text{div})\)-conforming LSFEM
Numerical Results

- shock flow: $u_{left} = 1.0$, $u_{right} = 0.5$, shock speed $s = 0.75$
- convergence to correct weak solution with optimal order
- no oscillations, correct shock speed, no CFL limit
Linear Advection – Higher-Order Elements

- order $k = 1, 2, 3, 4$: sharper shock for same dof
- remark: also discontinuous finite elements for $u^h$

(SIAM J. Sci. Comput., accepted)
Solution-Adaptive Refinement

- LS functional is sharp *a posteriori* error estimator:

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

- we minimize

\[
\mathcal{F}(\tilde{w}^h, u^h; g) = \|\nabla x,t \cdot \tilde{w}^h\|_{0,\Omega}^2 + \|\tilde{w}^h - \tilde{f}(u^h)\|_{0,\Omega}^2 \\
+ \|\tilde{n}_{x,t} \cdot (\tilde{w}^h - \tilde{f}(g))\|_{0,\Gamma_I}^2 + \|u^h - g\|_{0,\Gamma_I}^2
\]

- our \(H(div)\)-conforming LSFEM does not satisfy the exact discrete conservation property of Lax and Wendroff

\[
\nabla \cdot \tilde{w}^h
\]
Numerical Conservation

\[
F(w^h, u^h; g) = \| \nabla_{x,t} \cdot w^h \|_{0,\Omega}^2 + \| \vec{w}^h - \vec{f}(u^h) \|_{0,\Omega}^2 \\
+ \| \vec{n}_{x,t} \cdot (\vec{w}^h - \vec{f}(g)) \|_{0,\Gamma_I}^2 + \| u^h - g \|_{0,\Gamma_I}^2
\]

- however, we can prove: (submitted to SIAM J. Sci. Comput.)

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

If finite element approximation \( \hat{u}^h \) 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)
LSFEM for Nonlinear Hyperbolic PDEs: Status

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

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

- need efficient solvers for $Au = f$
(A) Soil Sedimentation (Civil Engineering)

with Gert Bartholomeeusen, Mechanical Engineering, University of Oxford

- settling column experiments: soil particles settle
- nonlinear waves, modeled by

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0$$
Soil Sedimentation

- experimental determination of flux function $f(u)$, nonconvex

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0$$

Flux, [mm/min]

<table>
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<th>Porosity, [-]</th>
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<td>0.84</td>
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(kaolinite soil suspension)
Soil Sedimentation

- simulation using flux function
- observation of compound shock waves = shock + sonic rarefaction
- new theory for transition between sedimentation and consolidation

(Proceedings of the 2002 Conference on Hyperbolic Systems)
(B) Bow Shock Flows in Solar-Terrestrial Plasmas

- supersonic solar wind plasma induces quasi-steady bow shock in front of earth’s magnetosphere
- plasma = gas + magnetic field \( B \)
- described by Magnetohydrodynamics (MHD), hyperbolic system
Recall: Gas Dynamics Bow Shock
Bow Shock Flows in Solar-Terrestrial Plasmas

- simulation:
  for large upstream $B$:
  multiple shock fronts!

- reason: MHD has multiple waves
- also: compound shocks (like in sedimentation application)

- predictive result:
  - not observed yet
  - confirmed in several other MHD codes
  - new spacecraft may allow observation
(C) Supersonic Outflow from Exoplanet Atmospheres

with Feng Tian, Brian Toon, Alex Pavlov, PAOS, CU Boulder

- extrasolar planets, as of 13 January 2004
  - 104 planetary systems
  - 119 planets
  - 13 multiple planet systems

- gas giants (‘hot Jupiters’)
- very close to star (∼ 0.05 AU)
⇒ supersonic hydrogen escape
  (like the solar wind), Euler
Supersonic Outflow from Exoplanet Atmospheres
Supersonic Outflow from Exoplanet Atmospheres
Supersonic Outflow from Exoplanet Atmospheres

- planet around HD209458
  - 0.67 Jupiter masses, 0.05 AU
  - hydrogen atmosphere and escape observed
    (Vidal-Madjar, Nature March 2003)
- Feng’s simulations show:
  - extent and temperature of Hydrogen atmosphere consistent with observations
  - atmosphere is stable (1% mass loss in 10 billion years)
- ‘Mercury-type’ planet with gas atmosphere would lose 10% of mass in 8.5 million years
Collaborators

- **LSFEM for Hyperbolic PDEs**
  
  Luke Olson, Tom Manteuffel, Steve McCormick
  
  *Applied Math, CU Boulder*

- **Fluid Dynamics Applications**
  
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  *Oxford*
  
  Feng Tian, Brian Toon, Alex Pavlov
  
  *PAOS, CU Boulder*