Least-Squares Finite Element Methods for Nonlinear Hyperbolic PDEs

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> University of Waterloo Tuesday, 20 January 2004

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

$$\frac{\partial}{\partial t} \left(\int_{\Omega} U \, dV \right) + \oint_{\partial \Omega} \vec{n} \cdot \vec{F}(U) \, dA = 0$$

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

$$\frac{\partial u}{\partial t} + \frac{\partial u^2/2}{\partial x} = 0$$

- 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

$$\oint_{\Gamma} \vec{n}_{x,t} \cdot \vec{f}_{x,t}(u) \ dl = 0$$

• L₂ scalar product

•
$$L_2$$
 norm

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

$$|f||_{0,\Omega} = \sqrt{\int_{\Omega} f^2 \, dx dt}$$

• space $H(div, \Omega)$

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

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

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



Weak Solutions: Discontinuities



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Numerical Approximation: Finite Differences

• derivatives \Rightarrow use truncated Taylor series expansion

$$\Rightarrow \left. \frac{\partial u}{\partial x} \right|_i = \frac{u_i - u_{i-1}}{\Delta x} + O(\Delta x)$$

• Burgers:
$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0 \implies \frac{u_{i,n+1}^h - u_{i,n}^h}{\Delta t} + u_{i,n}^h \frac{u_{i,n}^h - u_{i-1,n}^h}{\Delta x} = 0$$

- ⇒ convergence to wrong solution!
- reason: Taylor expansion not valid at shock!



Conservative Finite Difference Schemes



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

$$\oint_{\partial\Omega} \vec{n}_{x,t} \cdot \vec{f}_{x,t}(u) \ dl = 0$$

 $\Rightarrow \quad \text{exact discrete conservation in} \\ \text{every discrete cell } \Omega_i$



• exact discrete conservation constrains the solution, s.t. convergence to a solution with wrong shock speed cannot happen

Lax-Wendroff Scheme



• 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

$$u_*^h = \underset{u^h \in \mathcal{U}^h}{arg \min} \|\nabla_{x,t} \cdot \vec{f}_{x,t}(u^h)\|_{0,\Omega}^2$$

• goal:

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

\Rightarrow minimization:

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

• condition for u^h stationary point:

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

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} :

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

$$\nabla_{x,t} \cdot \vec{w} = 0 \qquad \qquad \Omega$$

$$\vec{w} = \vec{f}_{x,t}(u) \qquad \Omega$$

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

$$u = g$$
 Γ_I

• functional

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

• Newton linearization: minimize functional with linearized equation

- weak solution: $\vec{f}_{x,t} \in H(div, \Omega)$ \Rightarrow choose $\vec{w}^h \in H(div, \Omega)$
- Raviart-Thomas elements: the normal components of \vec{w}^h are continuous

 $\Rightarrow \vec{w}^h \in H(div, \Omega)$

 $\Rightarrow H(div)$ -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



Solution-Adaptive Refinement

• LS functional is sharp a posteriori error estimator:

$$\mathcal{F}(u^{h}) = \|Lu^{h}\|_{0,\Omega}^{2}$$

= $\|Lu^{h} - Lu_{exact}\|_{0,\Omega}^{2}$
= $\|L(u^{h} - u_{exact})\|_{0,\Omega}^{2}$
= $\|Le^{h}\|_{0,\Omega}^{2}$



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Numerical Conservation

• we minimize

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

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



Numerical Conservation

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

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

THEOREM. [Conservation for H(div)-conforming LSFEM] If finite element approximation d^h converges in the L_2 sense to \hat{u} as $h \rightarrow 0$, then \hat{u} is a weak solution of the conservation law.

⇒ 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

with Ulrike Yang, Center for Applied Scientific Computing, Lawrence Livermore National Laboratory

$$A u = f$$
 (n dof)

• scalable, or O(n), solver:

 \Rightarrow for a twice larger problem, you only need twice the work

 \Rightarrow 'optimal' solvers for sparse matrix problems

(not easy: Gaussian elimination $O(n^3)$...)

- parallel algebraic multigrid solvers
 - scalability for very large problems (\sim 1000s of processors)
 - scalability for hyperbolic PDEs

Scalable Linear Solvers



(3) Fluid Dynamics Applications



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

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

• experimental determination of flux function f(u), nonconvex

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



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) Driven Cavity Navier-Stokes Flow on Computational Grids



Computational Grids for Scientific Computing



- use several parallel computers at the same time (\sim power grid)
- developed Java-based grid computing framework

- applications:
 - fluid dynamics: driven cavity problem
 - iterative solver: scalable on grid
 - parallel bioinformatics problem (RNA folding)

(C) 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)

(Phys. Rev. Lett. 2000)

- predictive result:
- not observed yet
- confirmed in several other MHD codes
- new spacecraft may allow observation

Collaborators

- LSFEM for Hyperbolic PDEs
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 Tom Manteuffel
 Steve McCormick
 Applied Math, CU Boulder
 Scalable Solvers
 Ulrike Yang
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 John Ruge
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- Fluid Dynamics Applications
 Gert Bartholomeeusen, Thomas Pohl, Rob Markel
 Oxford, Erlangen, NCAR

Hyperbolic PDE Systems

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

• PDE of hyperbolic type: consider 1D

$$\frac{\partial U}{\partial t} + \frac{\partial F_x(U)}{\partial x} = 0 \qquad \text{or} \qquad \frac{\partial U}{\partial t} + \frac{\partial F_x(U)}{\partial U} \cdot \frac{\partial U}{\partial x} = 0$$

• define Flux Jacobian matrix G(U)

$$\mathbf{G}(U) = \frac{\partial F_x(U)}{\partial U}$$

- PDE is hyperbolic ⇐⇒ G(U) has real eigenvalues and a complete set of eigenvectors
- the eigenvalues λ_i of G(U) are wave speeds of the system, and define characteristic directions
- nonlinear waves can steepen into discontinuities: *shock waves*

Burgers Equation: Characteristic Curves



Numerical Results – Convergence Study

• solution regularity: $u \in H^{1/2-\epsilon} \quad \forall \epsilon > 0$ $\Rightarrow \|u - u^h\|_{0,\Omega} \leq c \ h^{1/2-\epsilon} \|u\|_{1/2-\epsilon,\Omega} \quad \forall \epsilon, \quad \text{optimally}$

• $\|u^h - u\|_{0,\Omega}^2 = O(h^{\alpha})$ and $\mathcal{F}(\vec{w}^h, u^h) = O(h^{\alpha})$, measure α

N	$\ u^h - u\ _{0,\Omega}^2$	lpha	$\mathcal{F}(\vec{w}^h, u^h)$	lpha
16	5.96e-3		1.89e-2	
32	3 81e-3	0.58	9 25e-3	1.03
		0.69		1.02
64	2.36e-3		4.56e-3	
128	1.38e-3	0.77	2.26e-3	1.01
256	7.66e-4	0.85	1.12e-3	1.01

Optimal O(n) **Solver: Multigrid Iterative Method**

• multigrid V-cycle:



- residual reduction per cycle: convergence factor $\rho = \frac{\|Au_{i+1} f\|}{\|Au_i f\|}$
- work per cycle $W_{1 \ cycle} = O(n)$

Optimal O(n) **Solver: Multigrid Method**





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Algebraic Multigrid Work in Progress

with Ulrike Yang, Center for Applied Scientific Computing, Lawrence Livermore National Laboratory

problem: hyperbolic PDEs: growth of convergence factor ρ as a function of n (not scalable)

processors	n (dof)	$ ho_{AMG}$
1	131,072	0.83
4	524,288	0.87
16	2,097,152	0.88
64	8,388,608	0.92
256	33,554,432	0.96
1,024	134,217,728	0.98

 $(256^2 \text{ nodes per processor})$

our approach: reformulate equations (SPD matrices), and more robust ways to choose coarse grids, interpolation matrix, relaxation

Scalable Nonlinear Solver – Newton Nested Iteration

- for many methods, number of Newton steps required grows with n
- use nested iteration:



Burgers: nested iteration with only one Newton step per level required!

(6) Scalable nonlinear solver – Newton FMG



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

(D) Supersonic Outflow from Exoplanet Atmospheres



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

- gas giants ('hot Jupiters')
- very close to star ($\sim 0.05~{\rm AU})$
- $\Rightarrow \ \text{supersonic hydrogen escape}$

(like the solar wind), Euler

Supersonic Outflow from Exoplanet Atmospheres



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Supersonic Outflow from Exoplanet Atmospheres



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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 12 billion years)
- 'Mercury-type' planet with gas atmosphere would lose
 10% of mass in 8.5 million years

(2) LSFEM for the Burgers equation

$$abla \cdot ec f(u) = 0 \quad \Omega
onumber \ u = g \quad \Gamma_I$$

• LS functional

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

• LSFEM

$$u^h_* = \underset{u^h \in \mathcal{U}^h}{\arg\min} \mathcal{H}(u^h; g)$$

LSFEM for the Burgers equation

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

 $u = g \quad \Gamma_{H}$

- 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



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



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:

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

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• 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



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 conservation



Hyperbolic PDEs – Conservation Laws

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

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

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

(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