

Least-Squares Finite Element Methods for Nonlinear Hyperbolic PDEs

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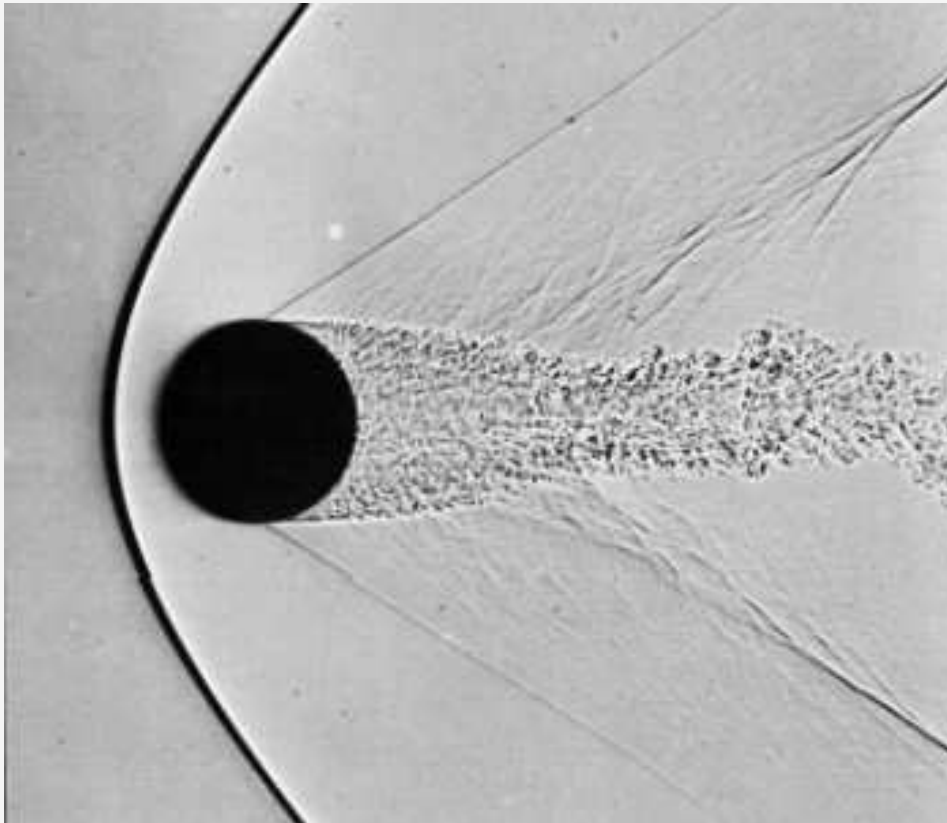
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Outline

- (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

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

Model Problem: Scalar Inviscid Burgers Equation

- scalar conservation law in 1D

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

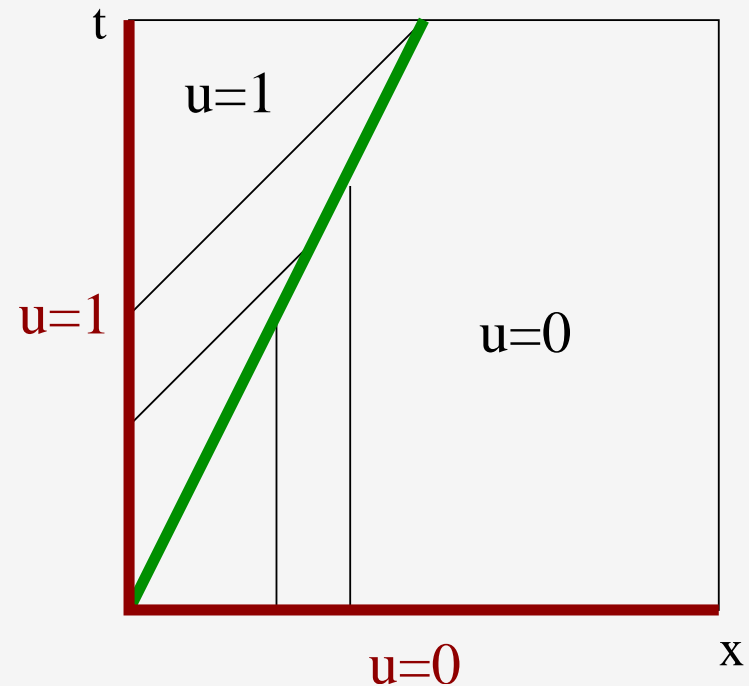
- model problem: inviscid Burgers equation

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

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

$$\begin{aligned}\nabla_{x,t} \cdot \vec{f}_{x,t}(u) &= 0 & \Omega \subset \mathbb{R}^2 \\ u &= g & \Gamma_I\end{aligned}$$

- 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

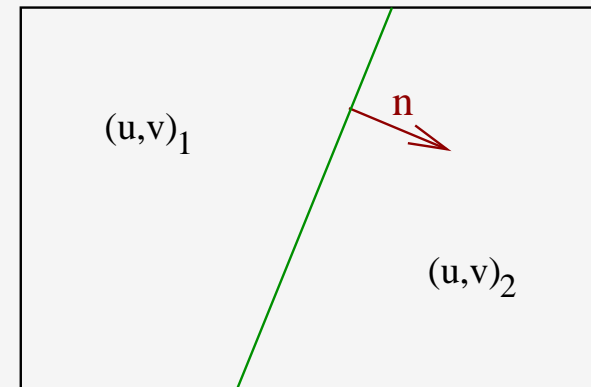
$$\|f\|_{0, \Omega} = \sqrt{\int_{\Omega} f^2 \, dx dt}$$

- space $H(\text{div}, \Omega)$

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

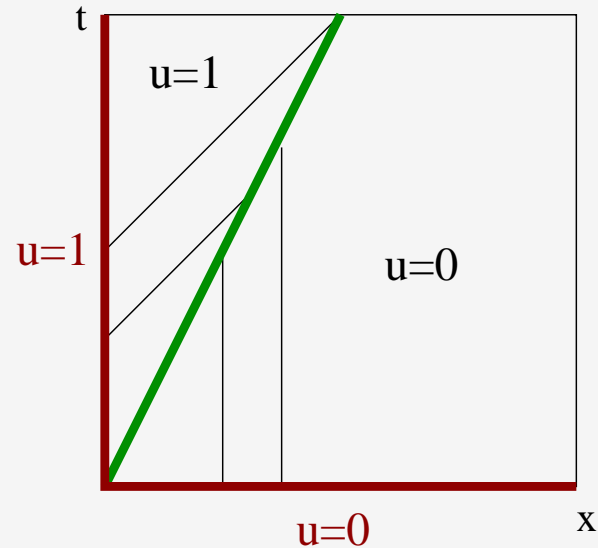
remark: (u, v) can be discontinuous,
with normal component continuous:

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



Weak Solutions: Discontinuities

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



(1) Rankine-Hugoniot relations: $\vec{n}_{x,t} \cdot (\vec{f}_{x,t}(u_2) - \vec{f}_{x,t}(u_1)) = 0$

(2) equivalent: $\vec{f}_{x,t}(u) \in H(\text{div}, \Omega)$ (solution regularity)

Burgers model flow: $\vec{f}_{x,t}(u) \in H(\text{div}, \Omega) \iff$ shock speed $s = \frac{1}{2}$

Numerical Approximation: Finite Differences

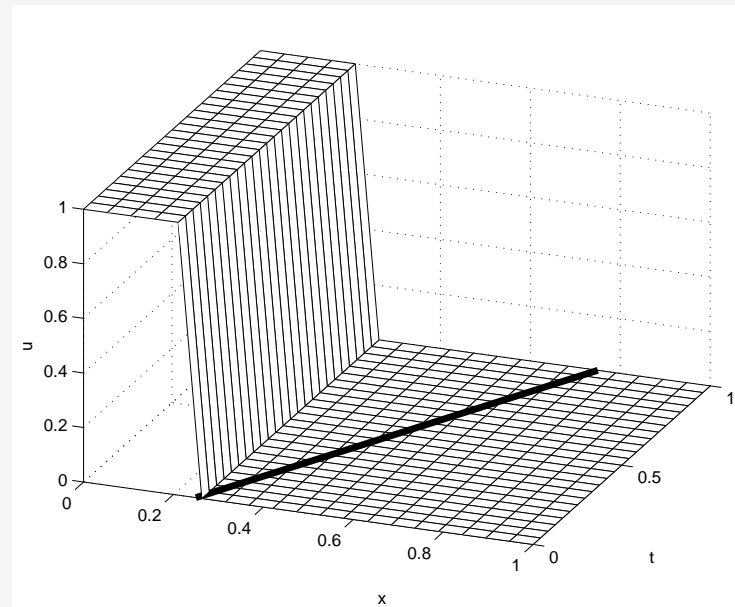
- derivatives \Rightarrow use truncated Taylor series expansion

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

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

\Rightarrow convergence to wrong solution!

- reason: Taylor expansion not valid at shock!

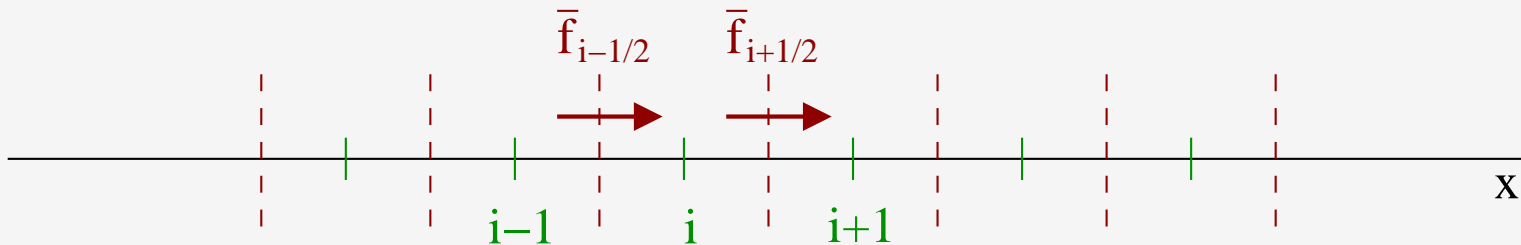


Conservative Finite Difference Schemes

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})



⇒ ‘conservative’ form is a *sufficient* condition for convergence to a weak solution (but it may not be *necessary!* ...)

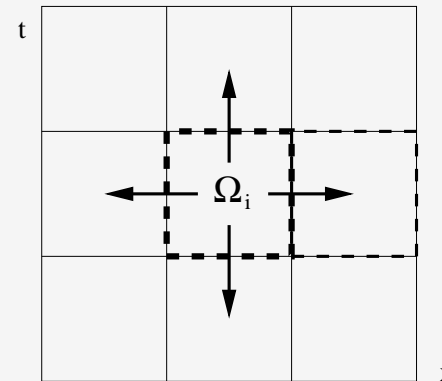
Why the Name ‘Conservative Scheme’?

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

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

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

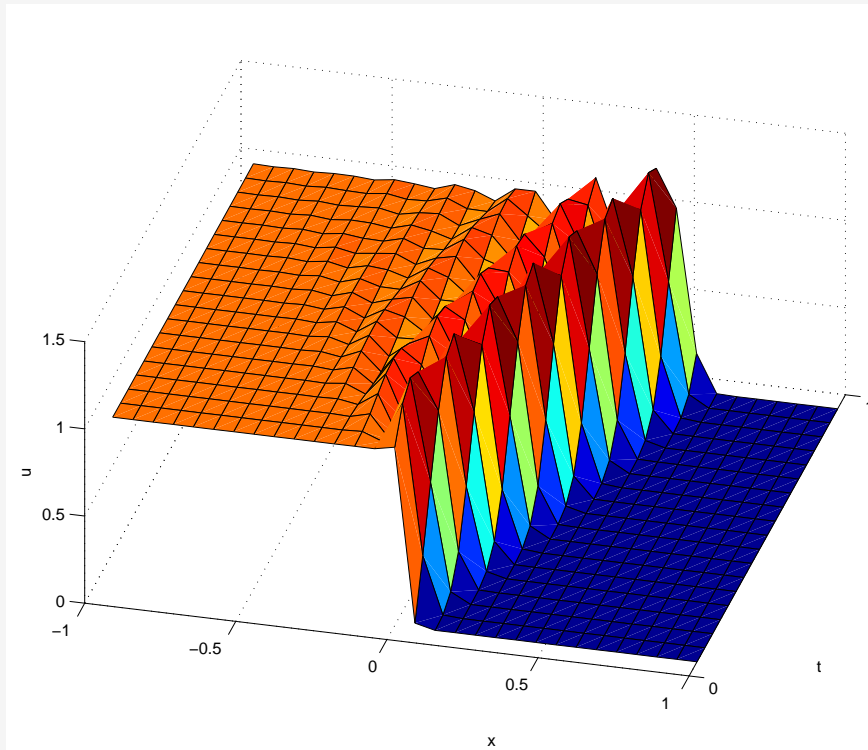
⇒ **exact discrete conservation** in every discrete cell Ω_i



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

Lax-Wendroff Scheme

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



- conservative
- $O(\Delta x^2)$ (Taylor)
- correct shock speed
- ... 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

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

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

⇒ achieve through norm minimization

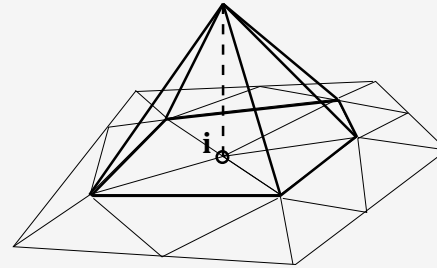
(remark: $h = \Delta x$)

(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:

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

- condition for u^h stationary point:

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

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, $A \mathbf{u} = 0$)

(actually, with boundary conditions, $A \mathbf{u} = \mathbf{f}$)

- **Symmetric Positive Definite (SPD)** matrices A

$H(\text{div})$ -Conforming LSFEM for Hyperbolic Conservation Laws

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

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

\Rightarrow

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

- functional

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

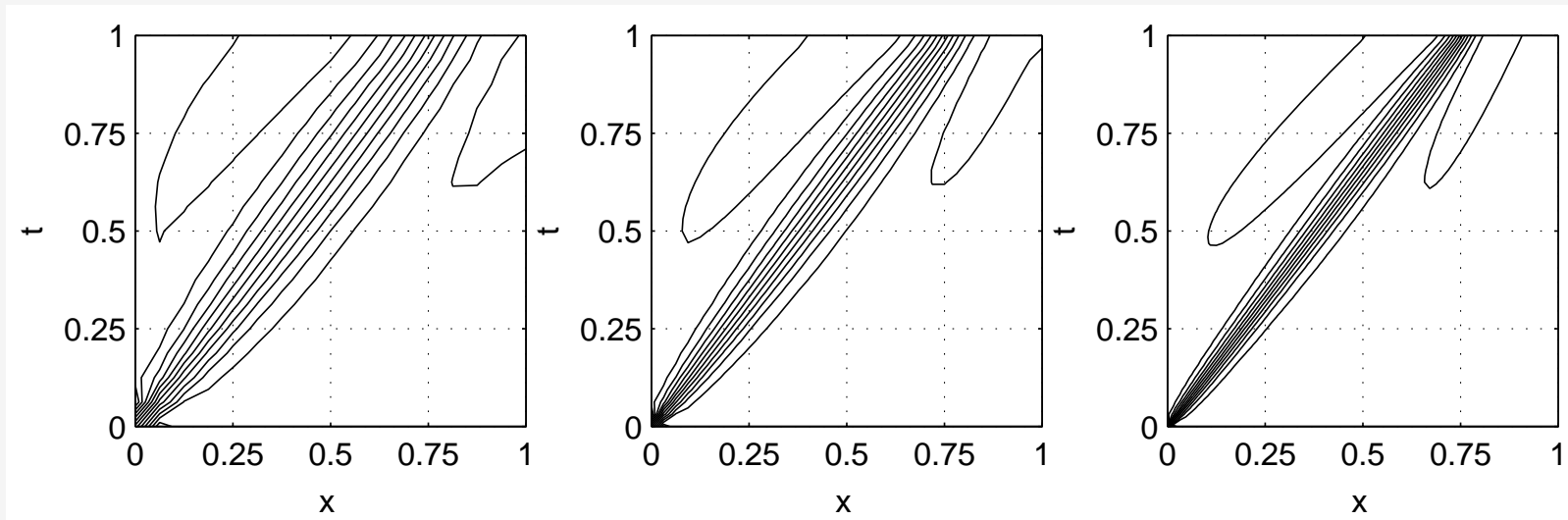
- Newton linearization:** minimize functional with linearized equation

Finite Element Spaces

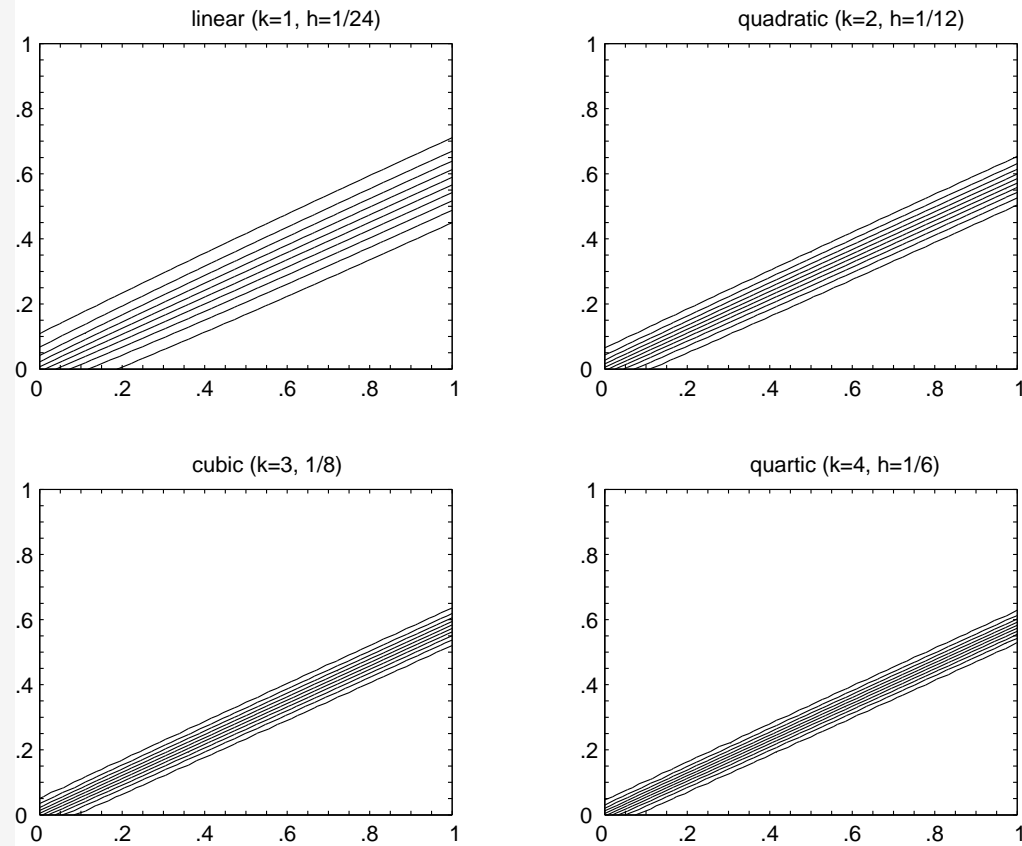
- weak solution: $\vec{f}_{x,t} \in H(\text{div}, \Omega)$
 \Rightarrow choose $\vec{w}^h \in H(\text{div}, \Omega)$
 - **Raviart-Thomas elements:** the normal components of \vec{w}^h are continuous
 $\Rightarrow \vec{w}^h \in H(\text{div}, \Omega)$
- $\Rightarrow H(\text{div})$ -conforming LSFEM

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

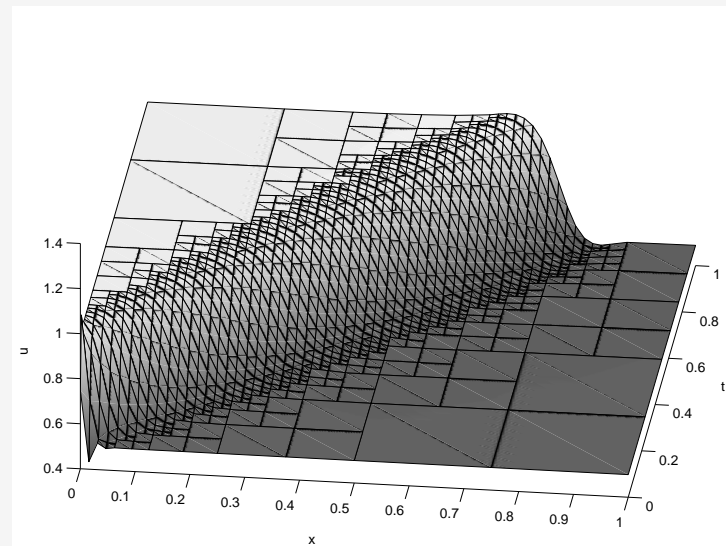
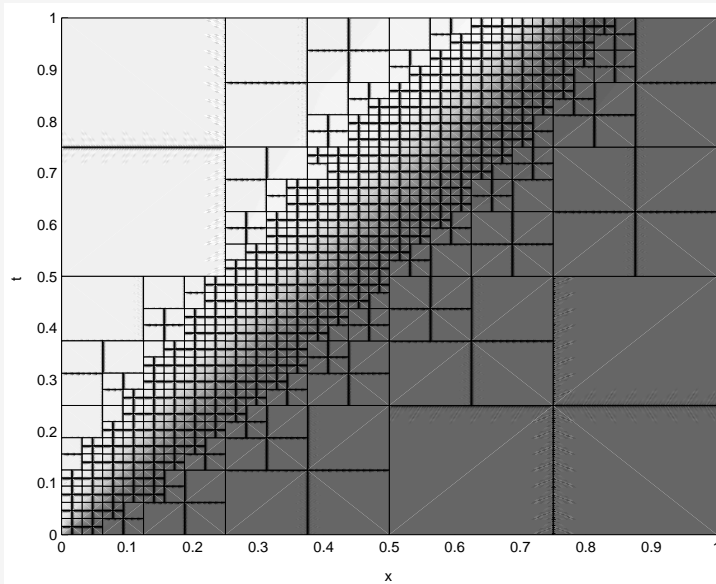


- order $k = 1, 2, 3, 4$: sharper shock for same dof
- remark: also discontinuous finite elements for u^h
(SIAM J. Sci. Comput., accepted)

Solution-Adaptive Refinement

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

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

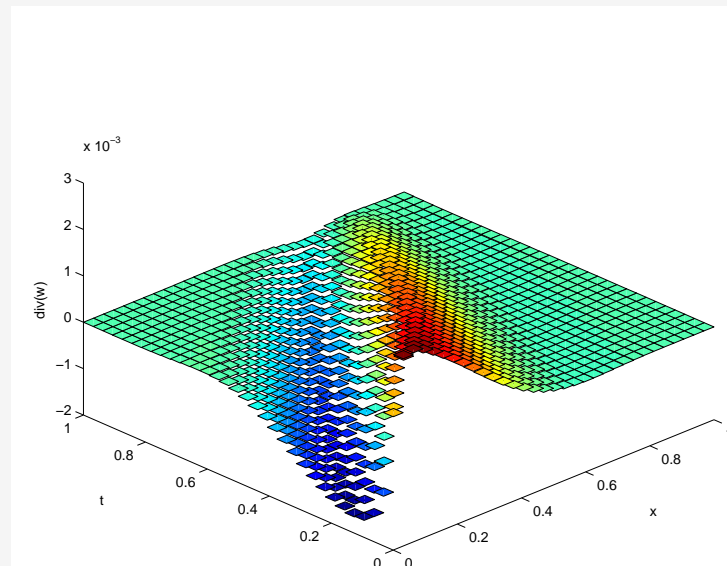


Numerical Conservation

- we minimize

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

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



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

Numerical Conservation

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

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

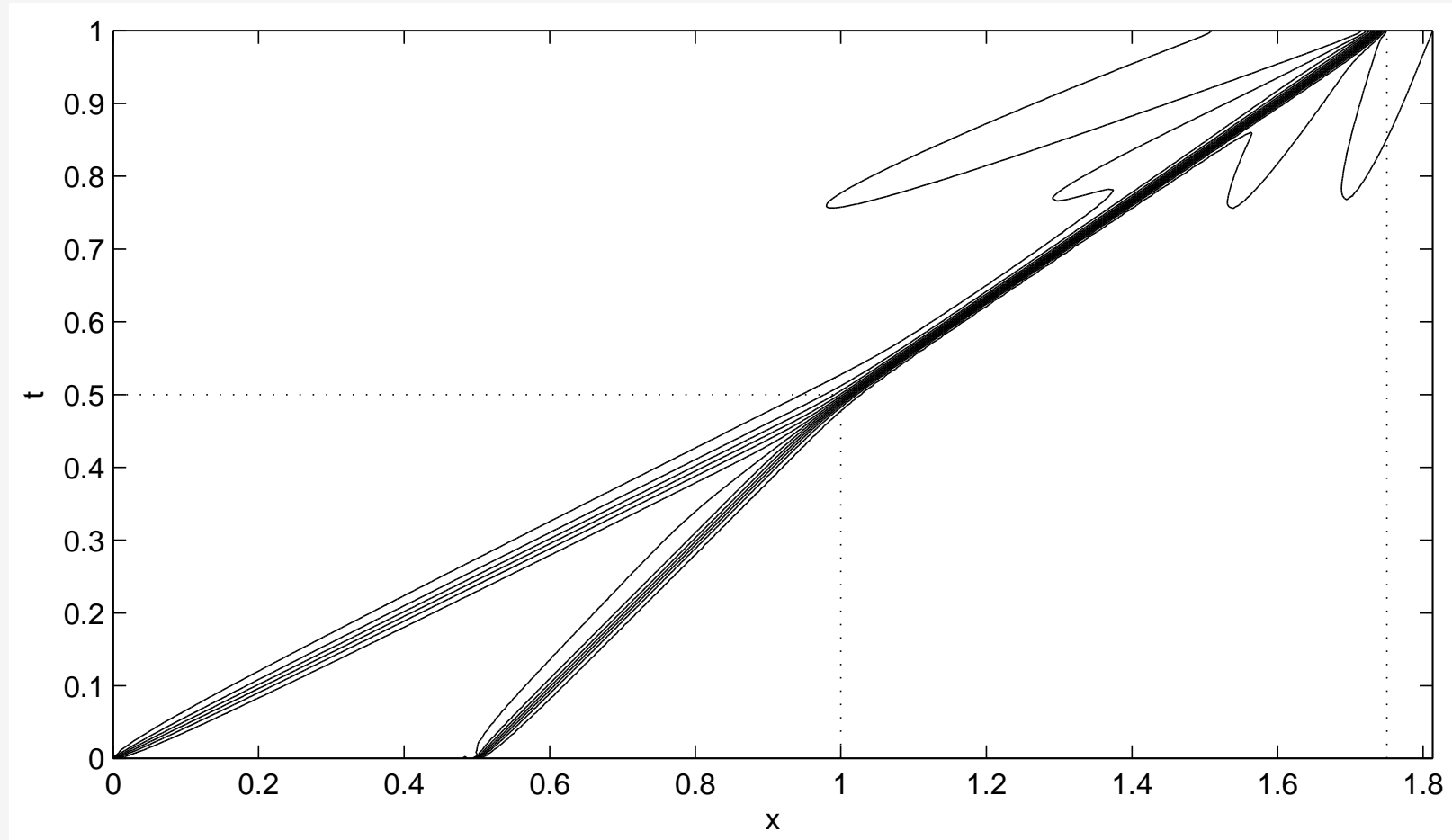
THEOREM. [Conservation for $H(\text{div})$ -conforming LSFEM]

If finite element approximation u^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)

Numerical conservation



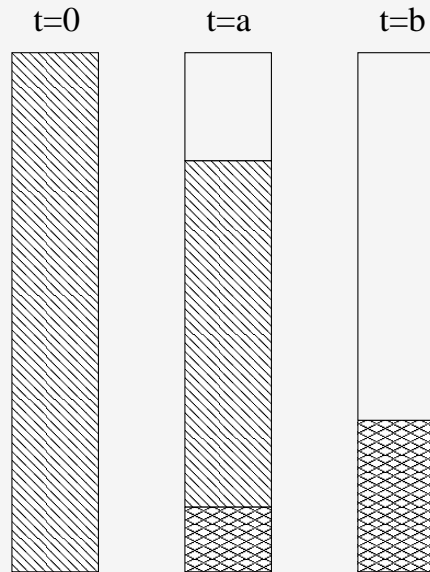
LSFEM for Nonlinear Hyperbolic PDEs: Status

- Burgers equation:
 - nonlinear
 - scalar
 - 2D domains
- extensions, in progress:
 - systems of equations
 - higher-dimensional domains
- need efficient solvers for $Au = f$

(3) Fluid Dynamics Applications

(A) Soil Sedimentation (Civil Engineering)

with Gert Bartholomeeusen, Mechanical Engineering, University of Oxford



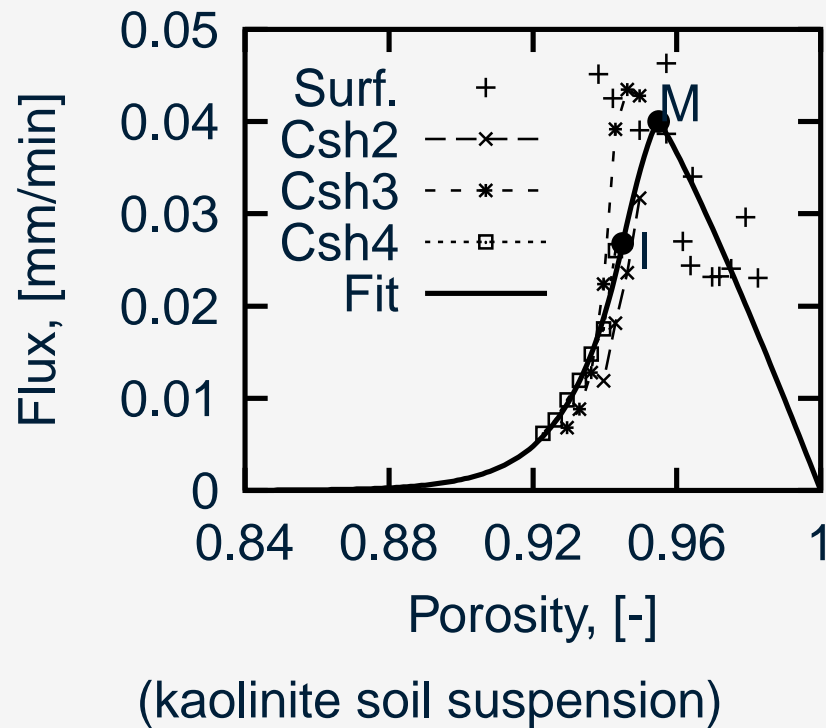
- settling column experiments: soil particles settle
- nonlinear waves, modeled by

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

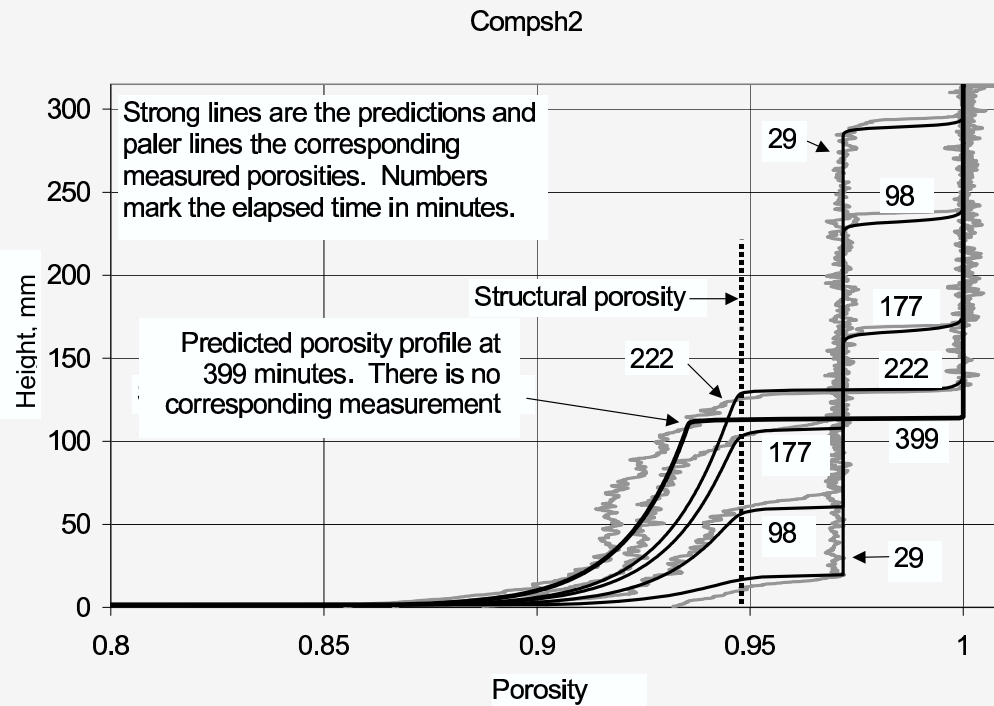
Soil Sedimentation

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

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

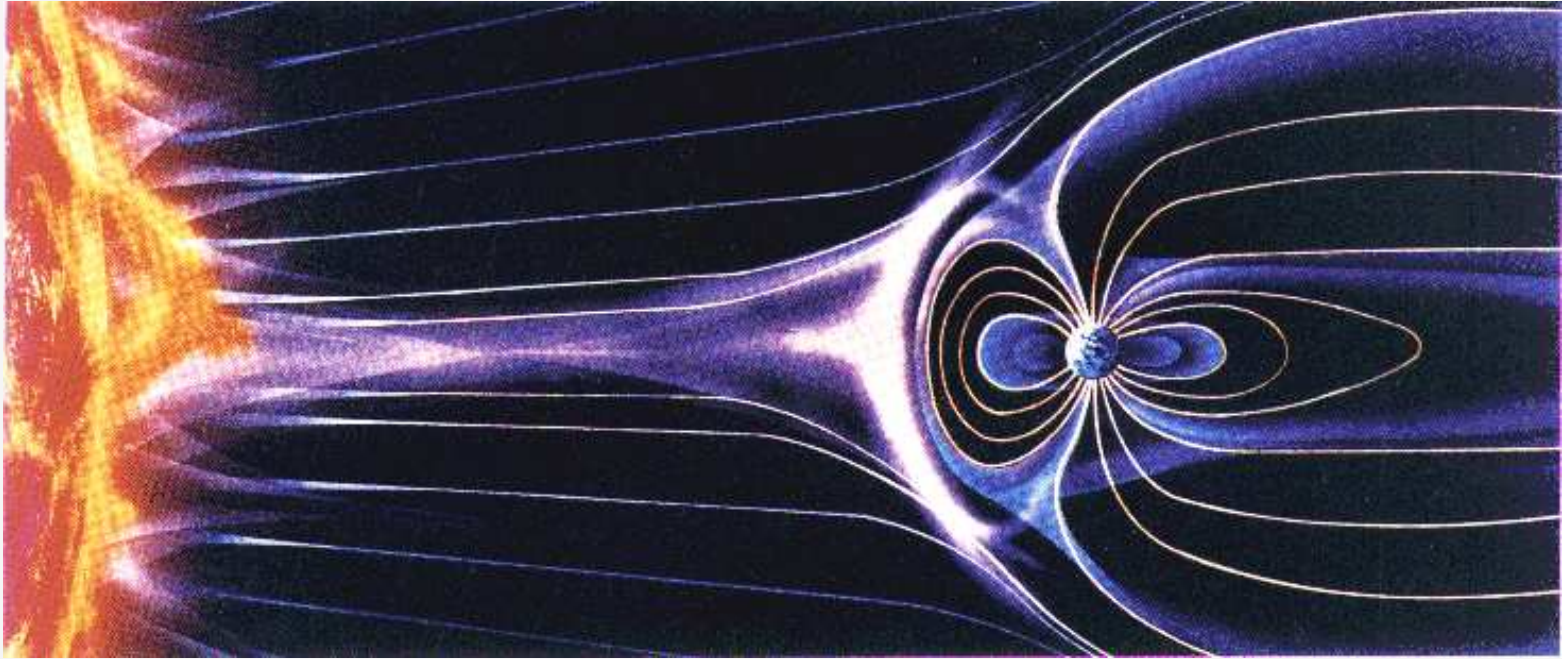


Soil Sedimentation



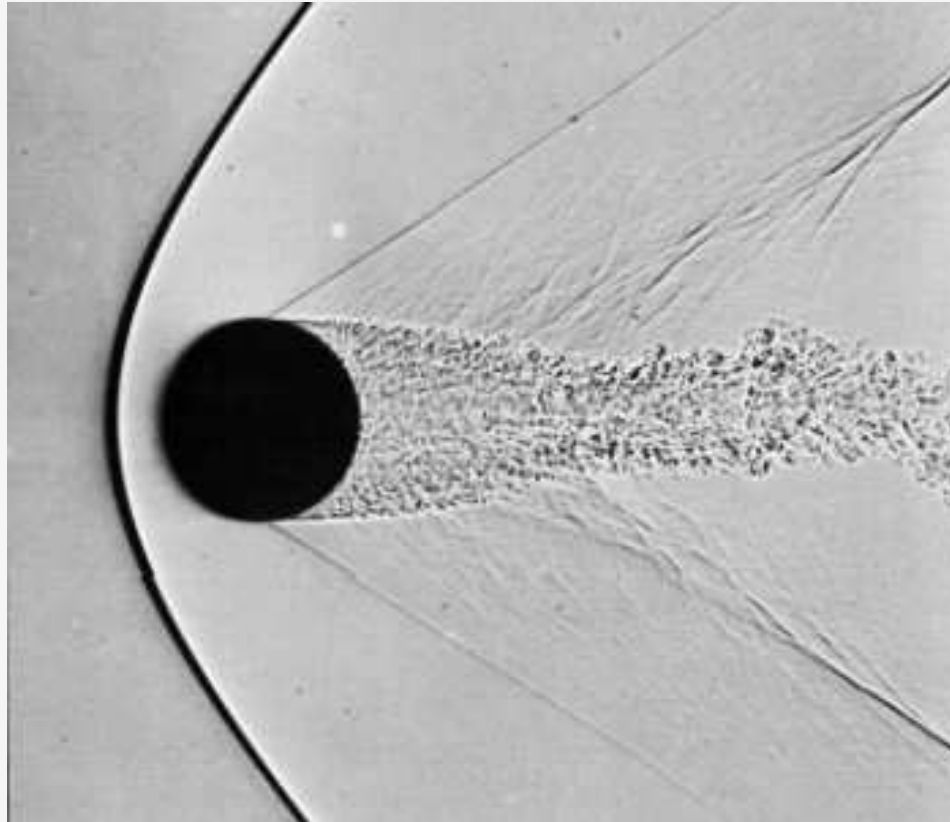
- simulation using flux function
 - observation of **compound shock waves** = shock + sonic rarefaction
 - **new theory** for transition between sedimentation and consolidation
- (Proceedings of the 2002 Conference on Hyperbolic Systems)

(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

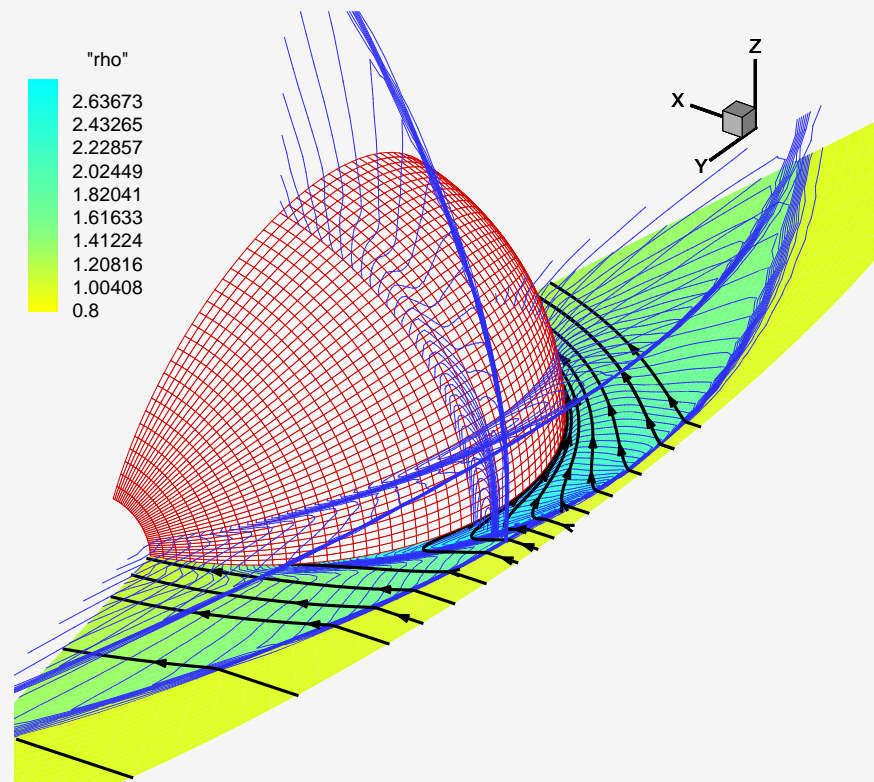


Bow Shock Flows in Solar-Terrestrial Plasmas

- **simulation:**

for large upstream B :

multiple shock fronts!



- reason: MHD has multiple waves

- also: **compound shocks** (like in sedimentation application)

(Phys. Rev. Lett. 2000)

- **predictive result:**

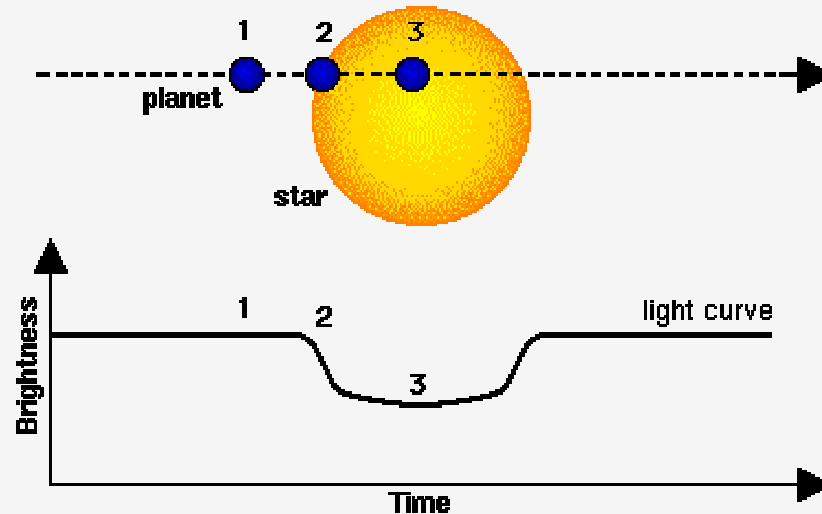
- not observed yet

- 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

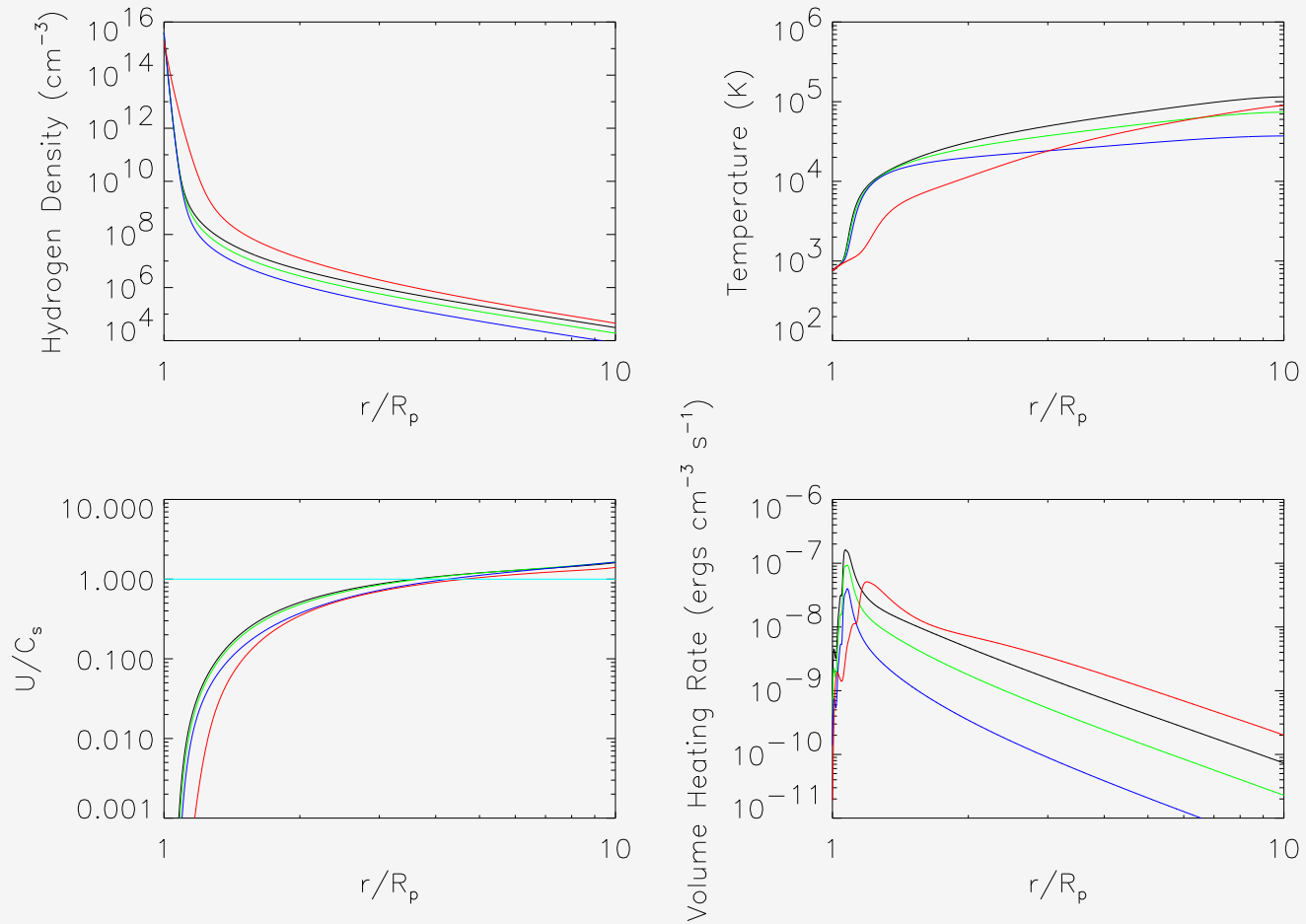


- extrasolar planets, as of 13 January 2004
 - 104 planetary systems
 - 119 planets
 - 13 multiple planet systems
 - gas giants ('hot Jupiters')
 - very close to star (~ 0.05 AU)
- \Rightarrow supersonic hydrogen escape
(like the solar wind), Euler

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

Gert Bartholomeeusen

Oxford

Feng Tian, Brian Toon, Alex Pavlov

PAOS, CU Boulder