Least-Squares Finite Element Methods for Nonlinear Hyperbolic PDEs

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APPM Colloquium

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Outline

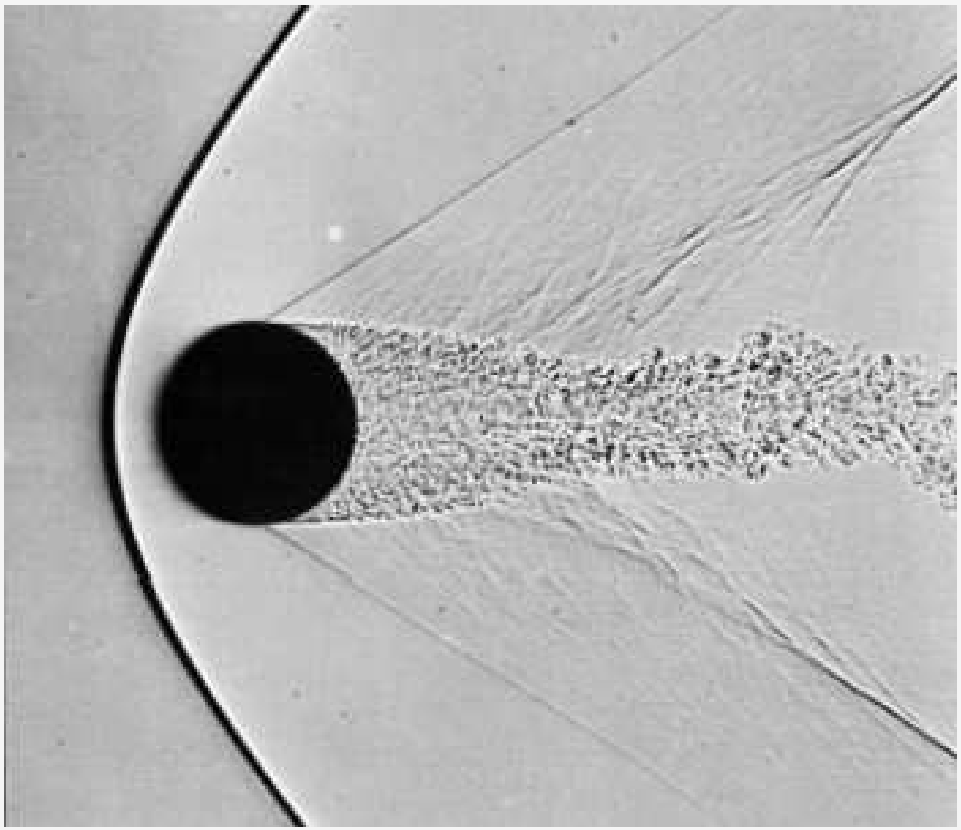
(1) Hyperbolic Conservation Laws: Introduction

(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

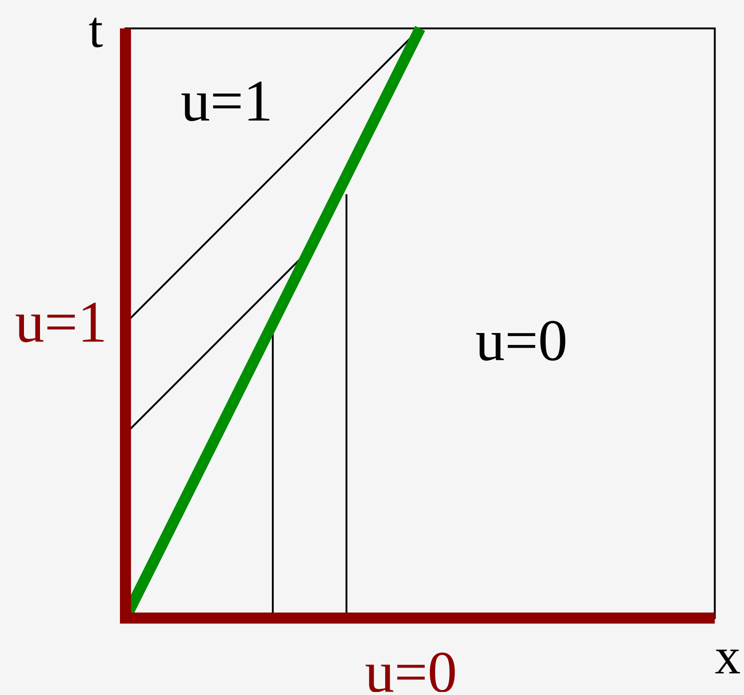
$$\frac{\partial u}{\partial t} + \frac{\partial u^2/2}{\partial x} = 0$$

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

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

- conservation in space-time

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

Some Notation

- L_2 scalar product

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

- L_2 norm

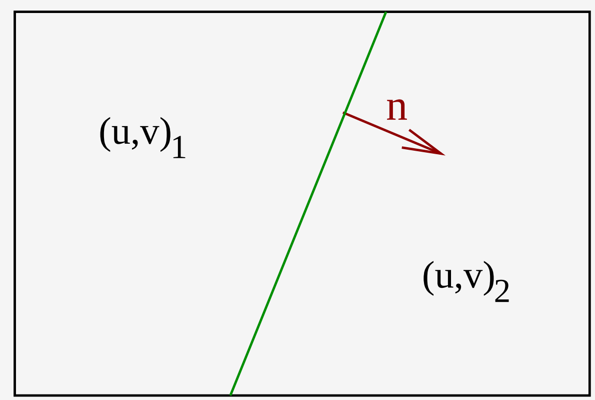
$$\|f\|_{0,\Omega} = \sqrt{\int_\Omega f^2\; dxdt}$$

- space $H(div, \Omega)$

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

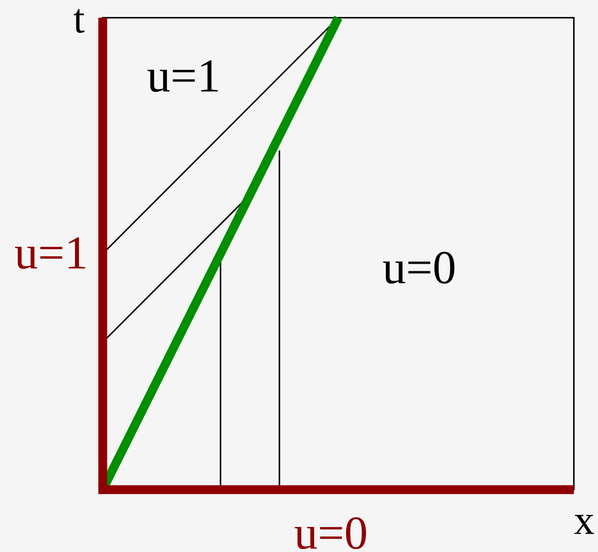
remark: (u,v) can be discontinuous, with normal component continuous:

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



Weak Solutions: Discontinuities

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



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

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

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

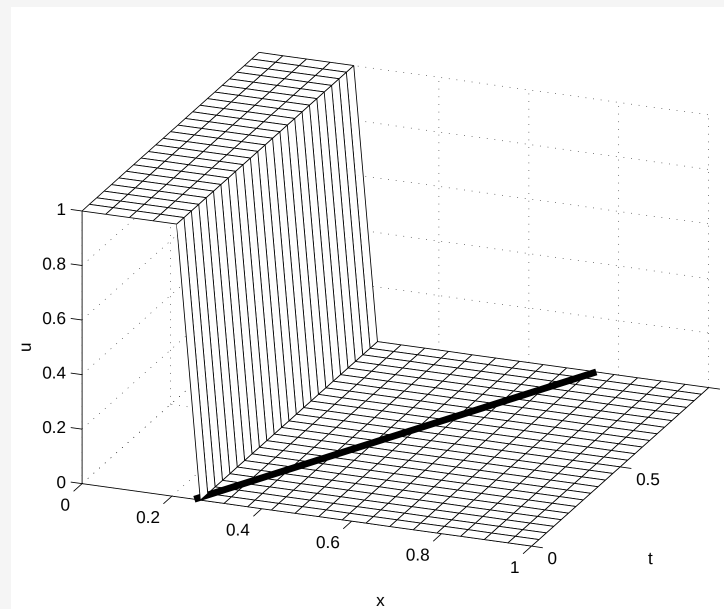
Numerical Approximation: Finite Differences

- 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: $\dfrac{\partial u}{\partial t} + u\dfrac{\partial u}{\partial x} = 0 \quad \Rightarrow \quad \dfrac{u^h_{i,n+1} - u^h_{i,n}}{\Delta t} + u^h_{i,n}\dfrac{u^h_{i,n} - u^h_{i-1,n}}{\Delta x} = 0$

$\Rightarrow$ convergence to wrong solution!



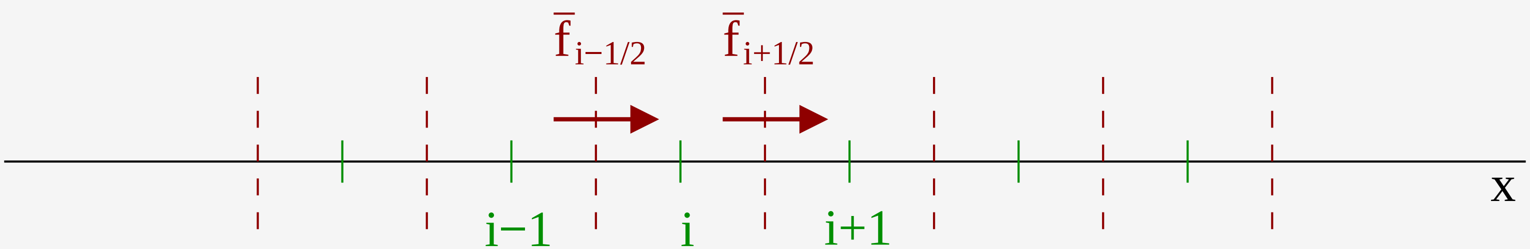
- reason: Taylor expansion not valid at shock!

Conservative Finite Difference Schemes

THEOREM. Lax-Wendroff (1960).

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

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



$\Rightarrow$ 'conservative' form is a *sufficient* condition for convergence to a weak solution (but it may not be *necessary*! . . .)

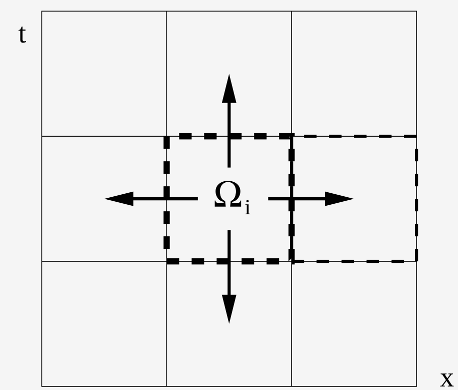
Why the Name 'Conservative Scheme'?

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

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

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

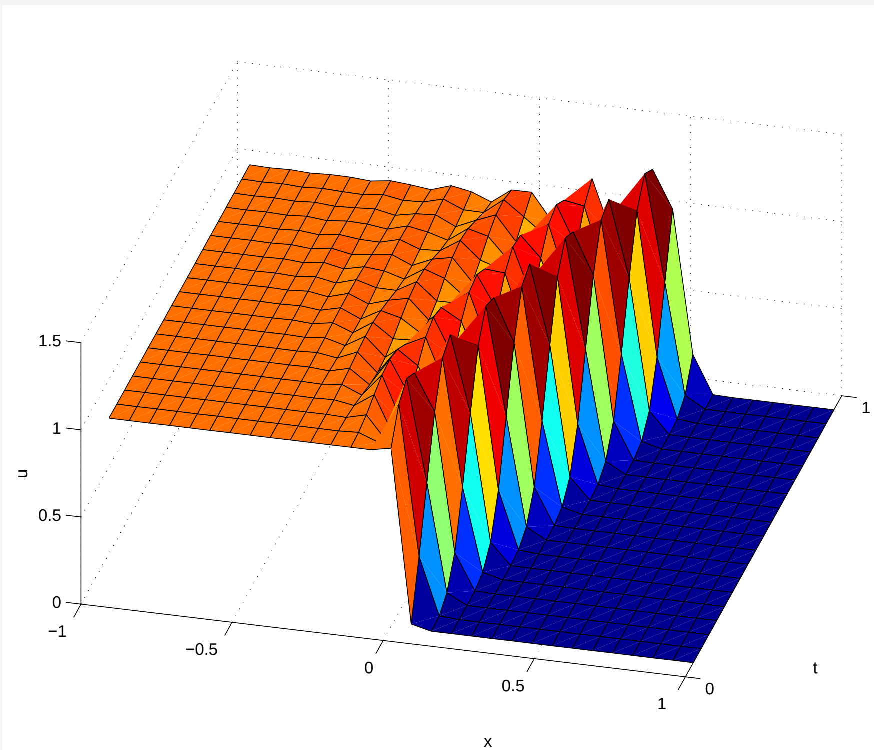
$\Rightarrow$ exact discrete conservation in every discrete cell Ω_i



- 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

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

- 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

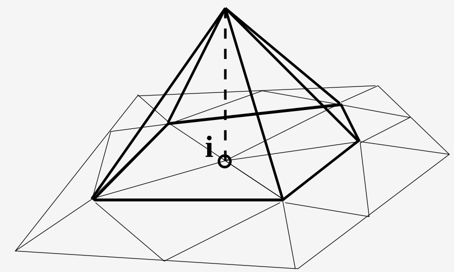
(remark: $h = \Delta x$)

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

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:

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

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

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

- Symmetric Positive Definite (SPD) matrices A

$H(div)$-Conforming LSFEM for Hyperbolic Conservation Laws

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

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

- 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: $\vec{f}_{x,t} \in H(div, \Omega)$

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

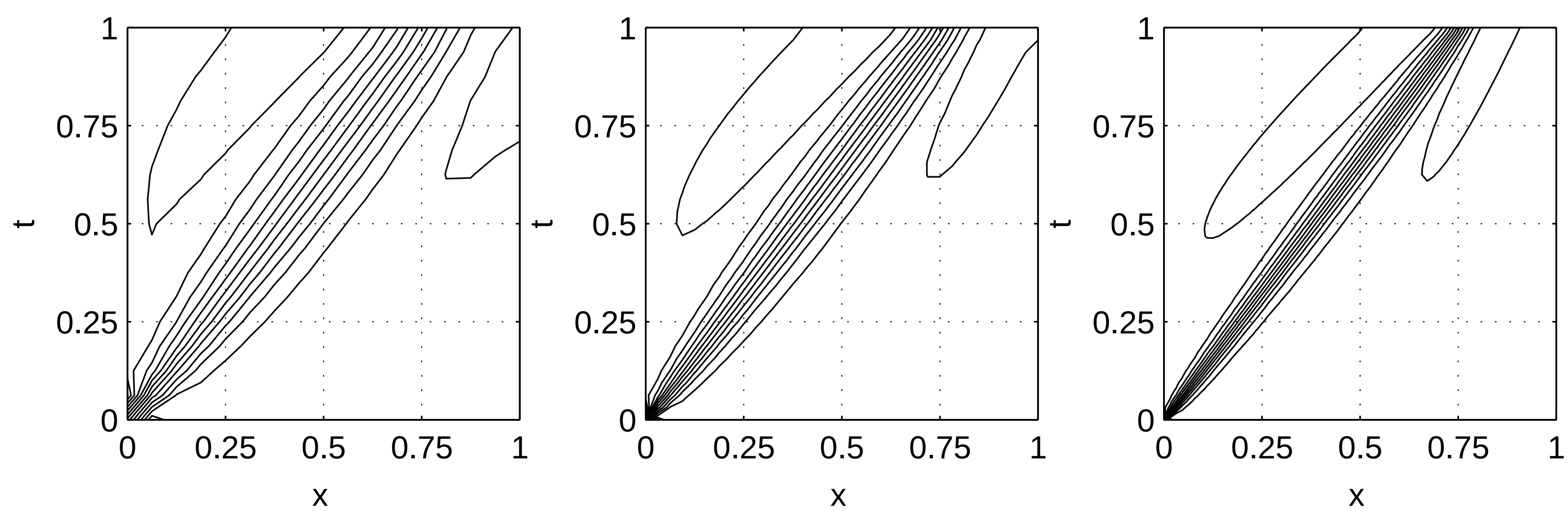
- Raviart-Thomas elements: the normal components of $\vec{w}^h$ are continuous

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

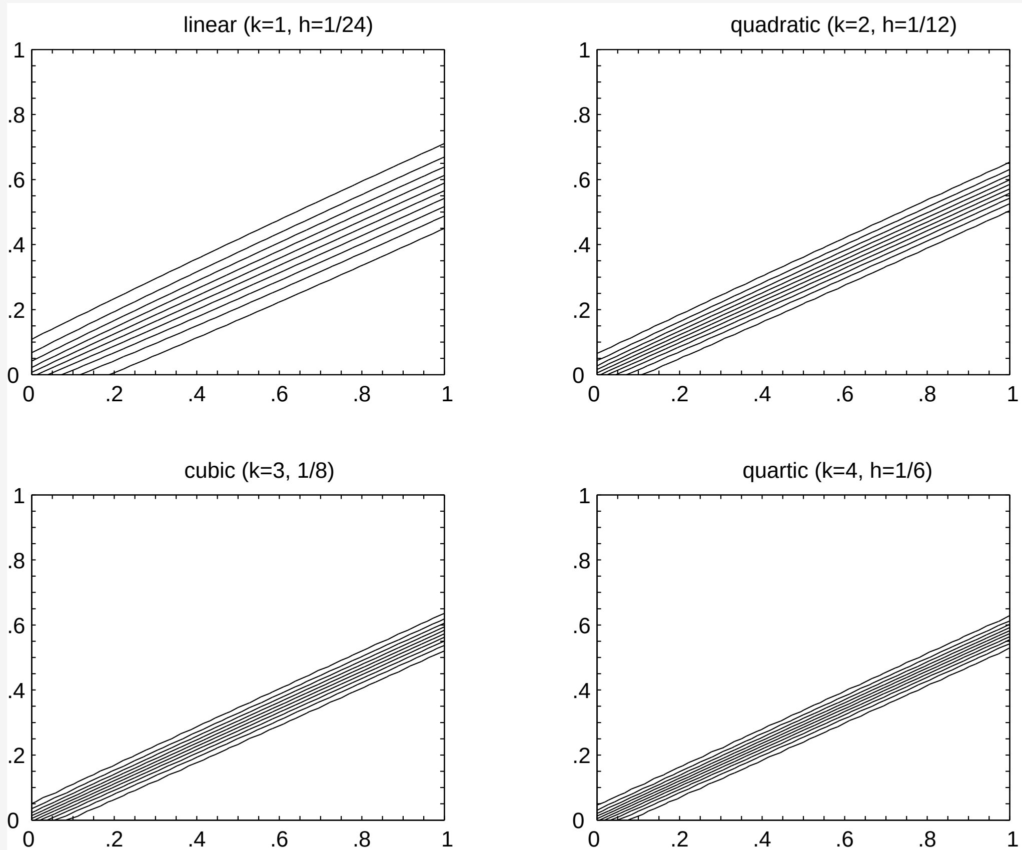
$\Rightarrow$ $H(div)$-conforming LSFEM

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



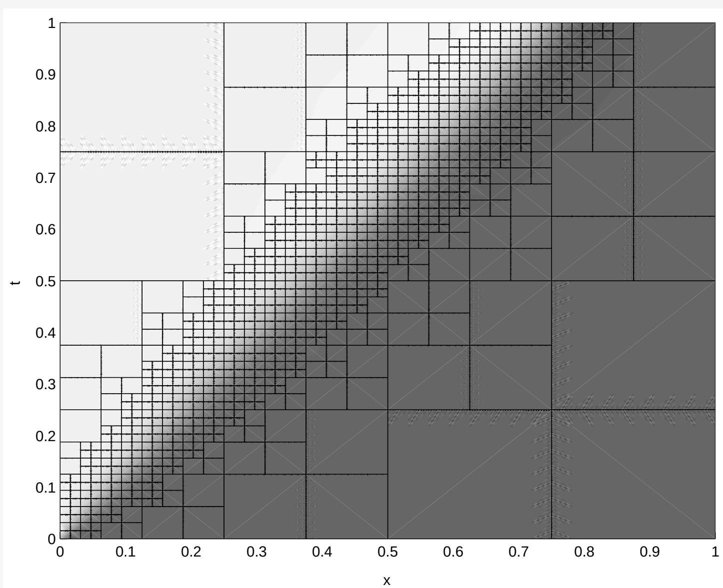
- order $k = 1,\ 2,\ 3,\ 4$: sharper shock for same dof
- remark: also discontinuous finite elements for u^h

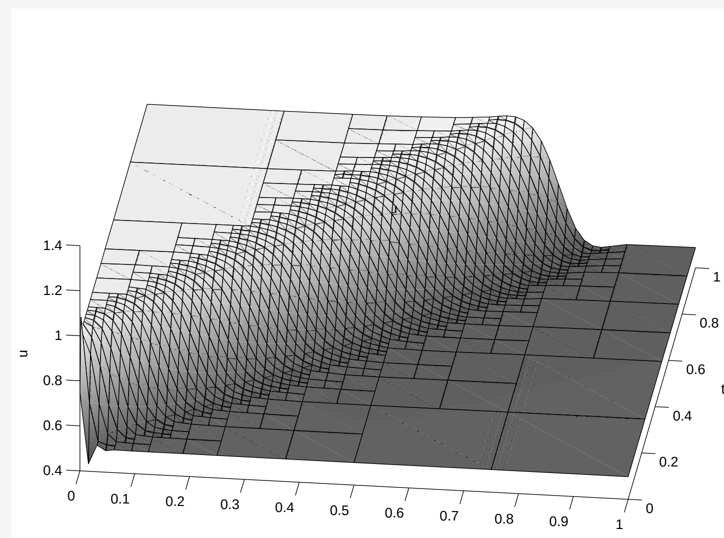
  (SIAM J. Sci. Comput., accepted)

Solution-Adaptive Refinement

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

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



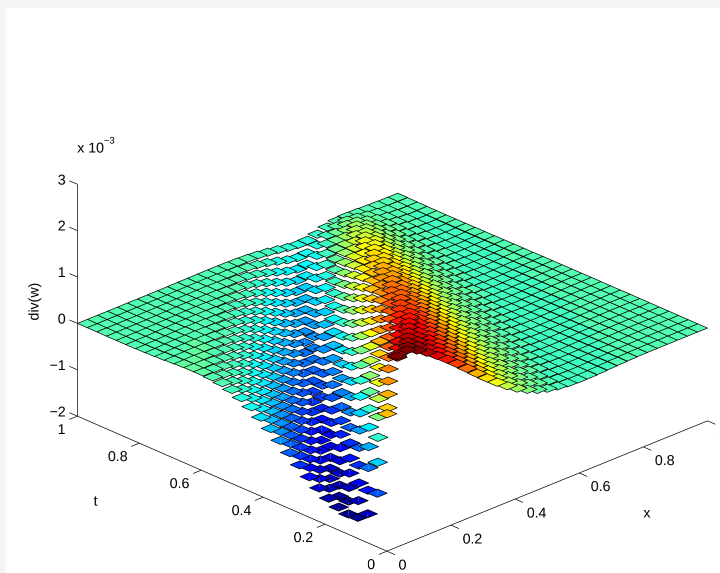


Numerical Conservation

- we minimize

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

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



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

Numerical Conservation

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

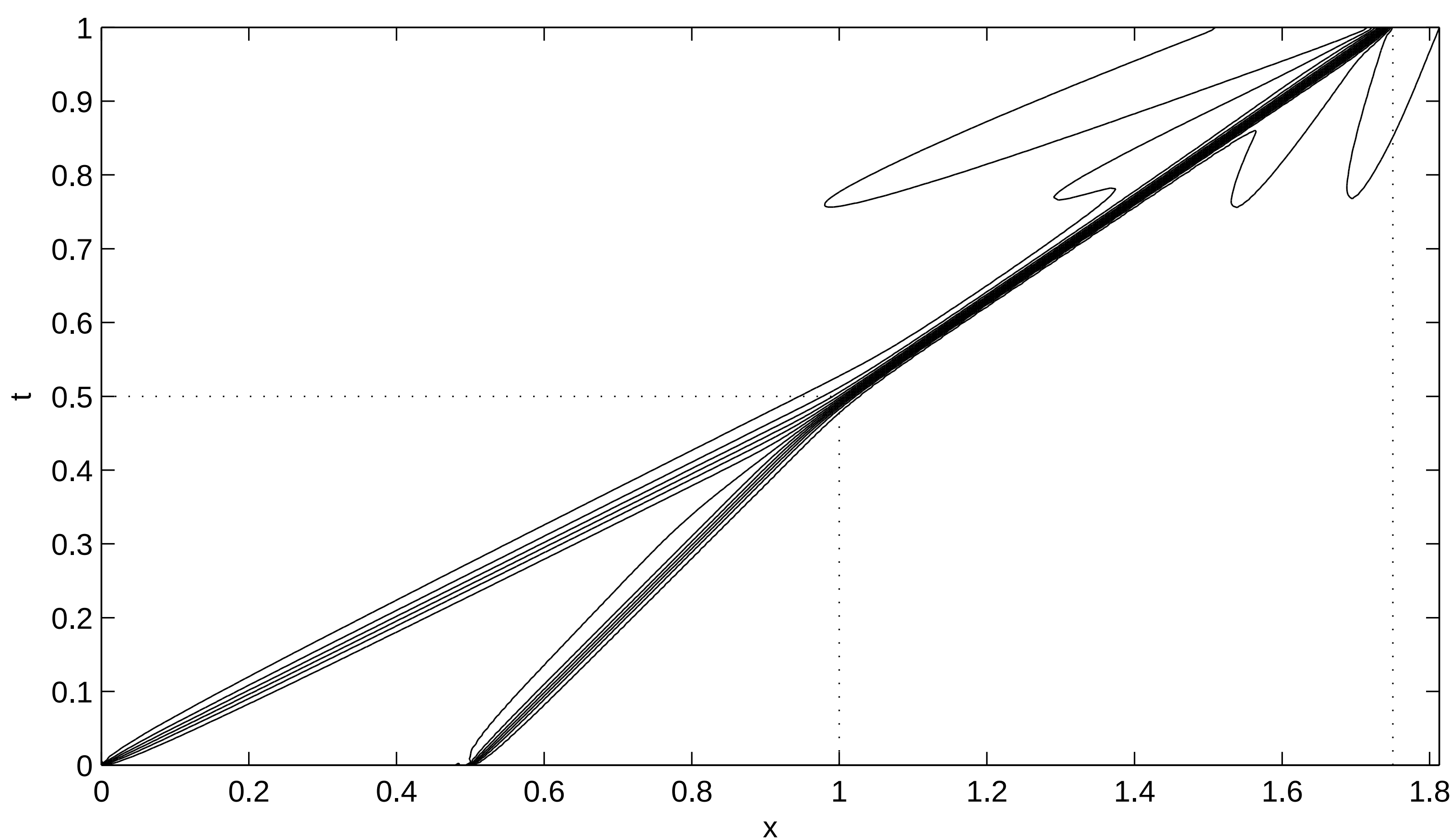
- however, we can prove: (submitted to SIAM J. Sci. Comput.)

THEOREM. [Conservation for $H(div)$-conforming LSFEM]
If finite element approximation 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)

Numerical conservation



LSFEM for Nonlinear Hyperbolic PDEs: Status

- Burgers equation:

  - nonlinear

  - scalar

  - 2D domains

- extensions, in progress:

  - systems of equations

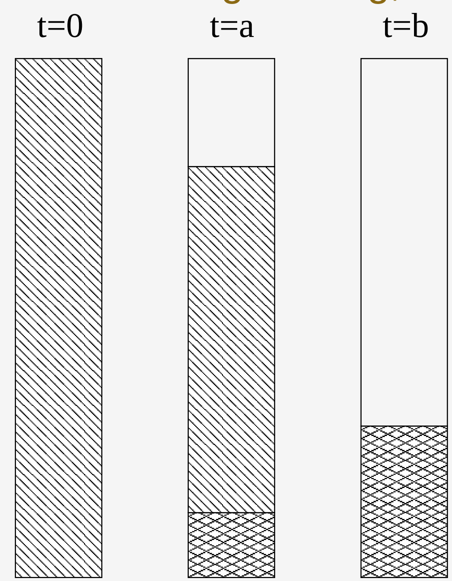
  - higher-dimensional domains

- need efficient solvers for $A u = f$

(3) Fluid Dynamics Applications

(A) Soil Sedimentation (Civil Engineering)

with Gert Bartholomeeusen, Mechanical Engineering, University of Oxford



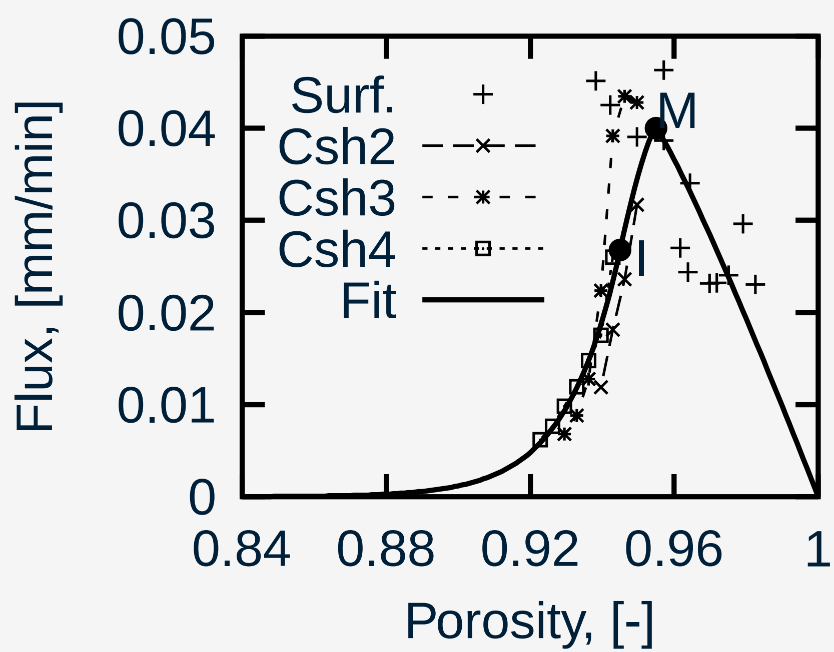
- settling column experiments: soil particles settle
- nonlinear waves, modeled by

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

Soil Sedimentation

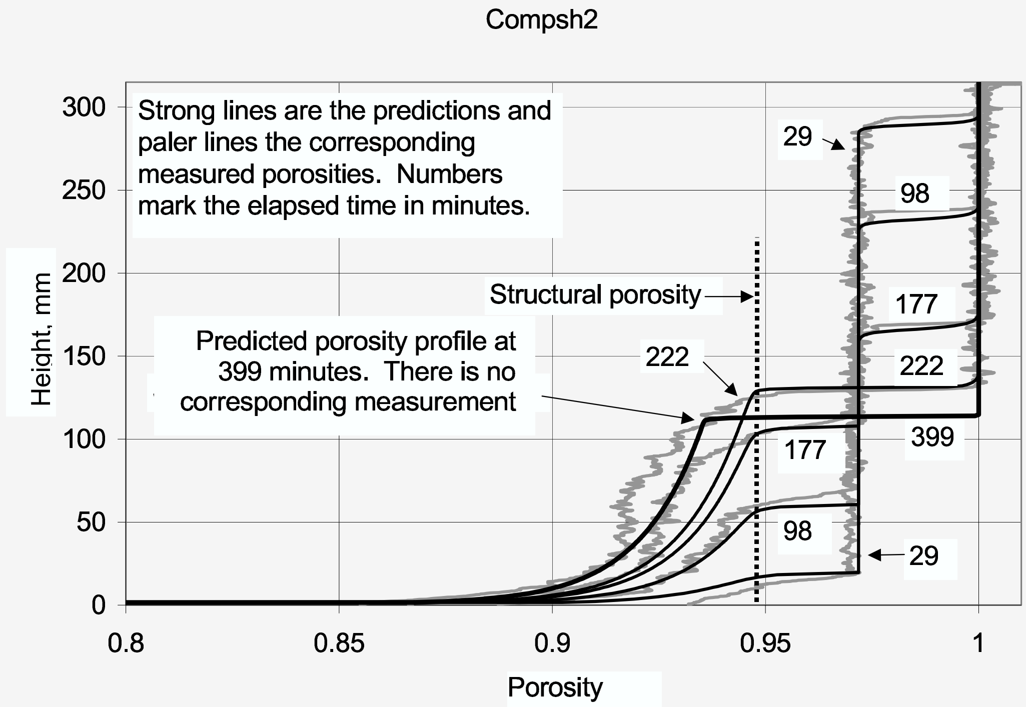
- experimental determination of flux function $f(u)$, nonconvex

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



(kaolinite soil suspension)

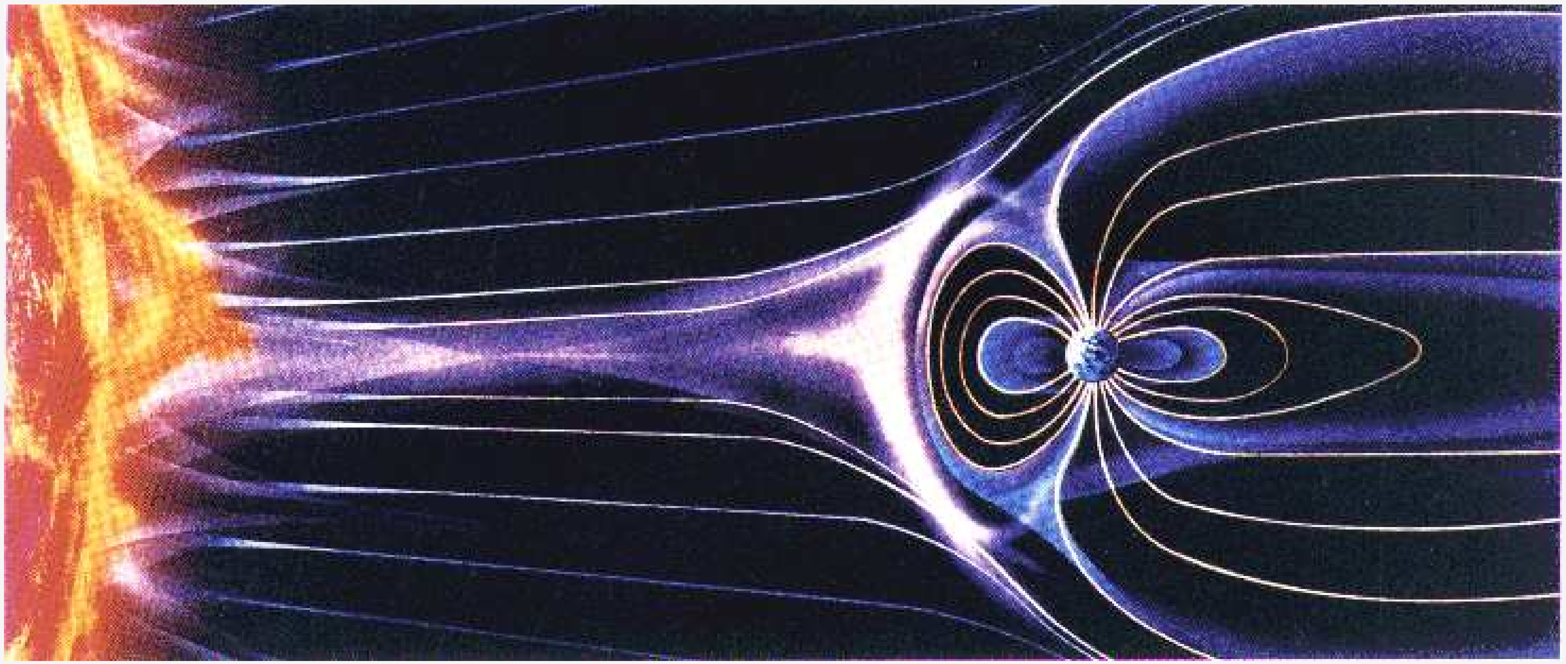
Soil Sedimentation



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

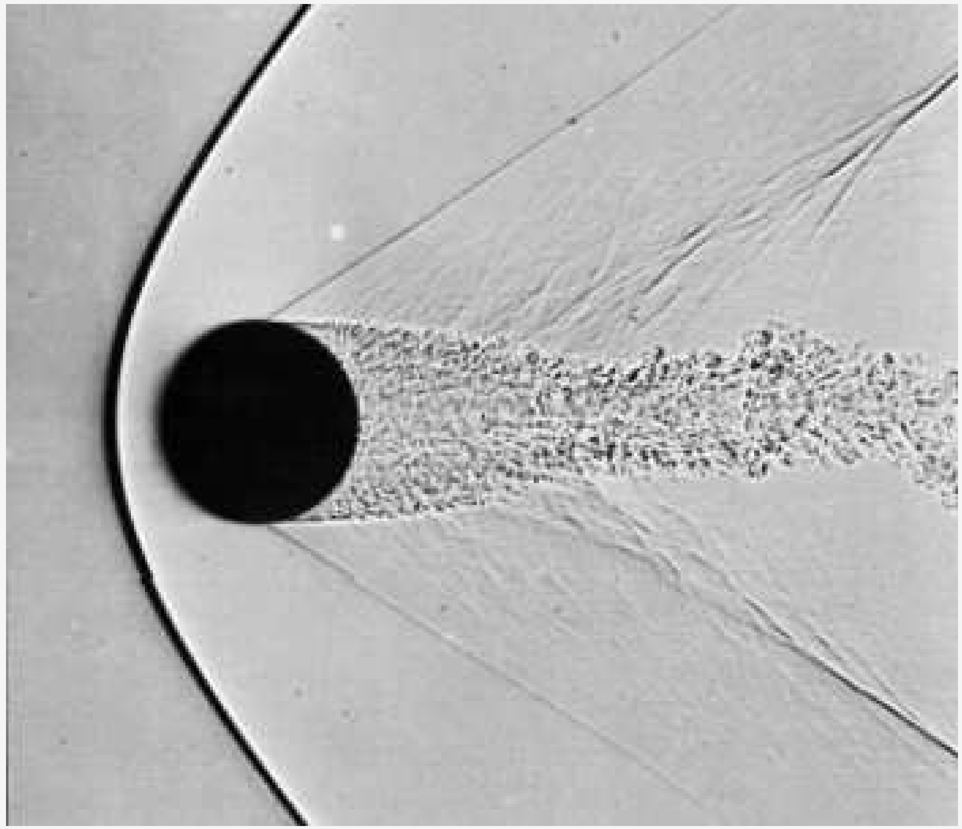
(Proceedings of the 2002 Conference on Hyperbolic Systems)

(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

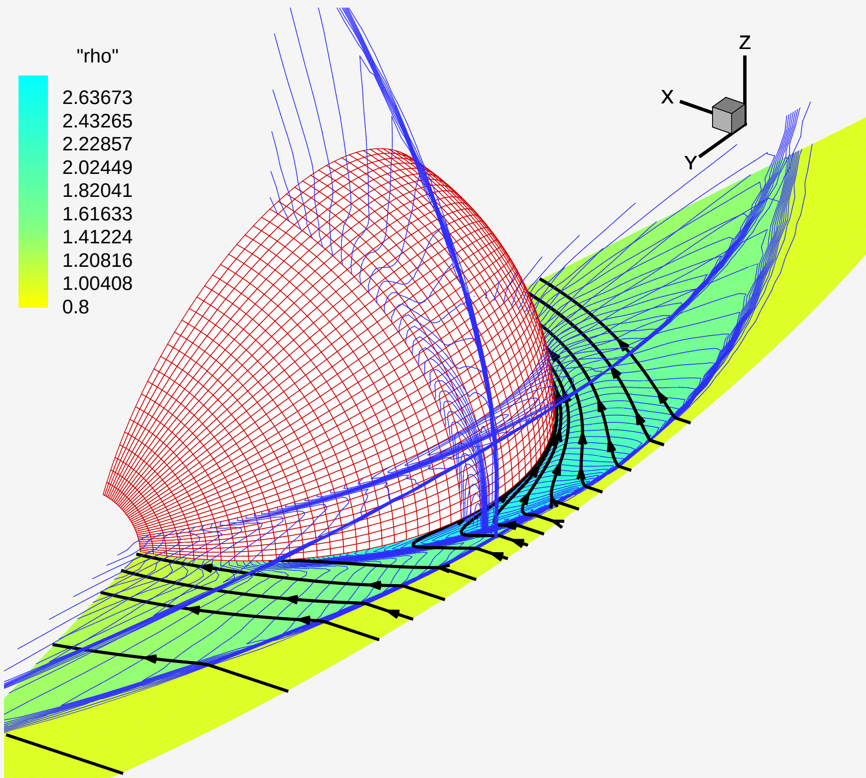


Bow Shock Flows in Solar-Terrestrial Plasmas

- simulation:

  for large upstream B:

  multiple shock fronts!



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

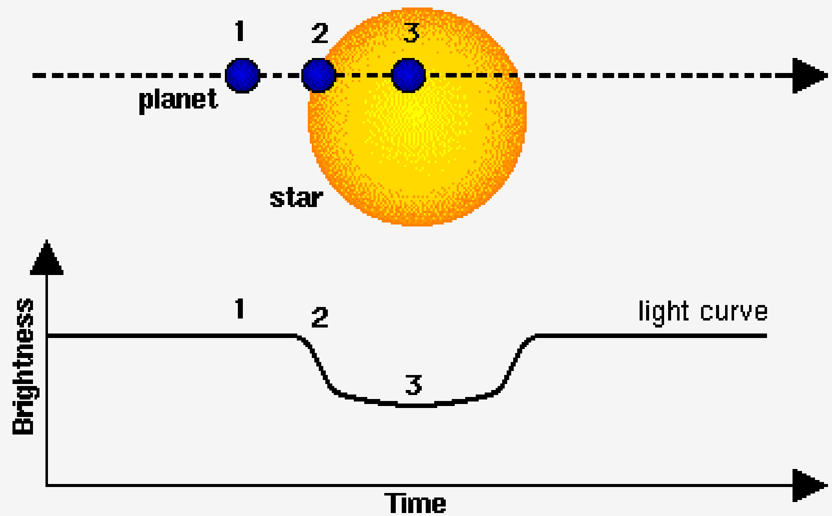
  (Phys. Rev. Lett. 2000)

- 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

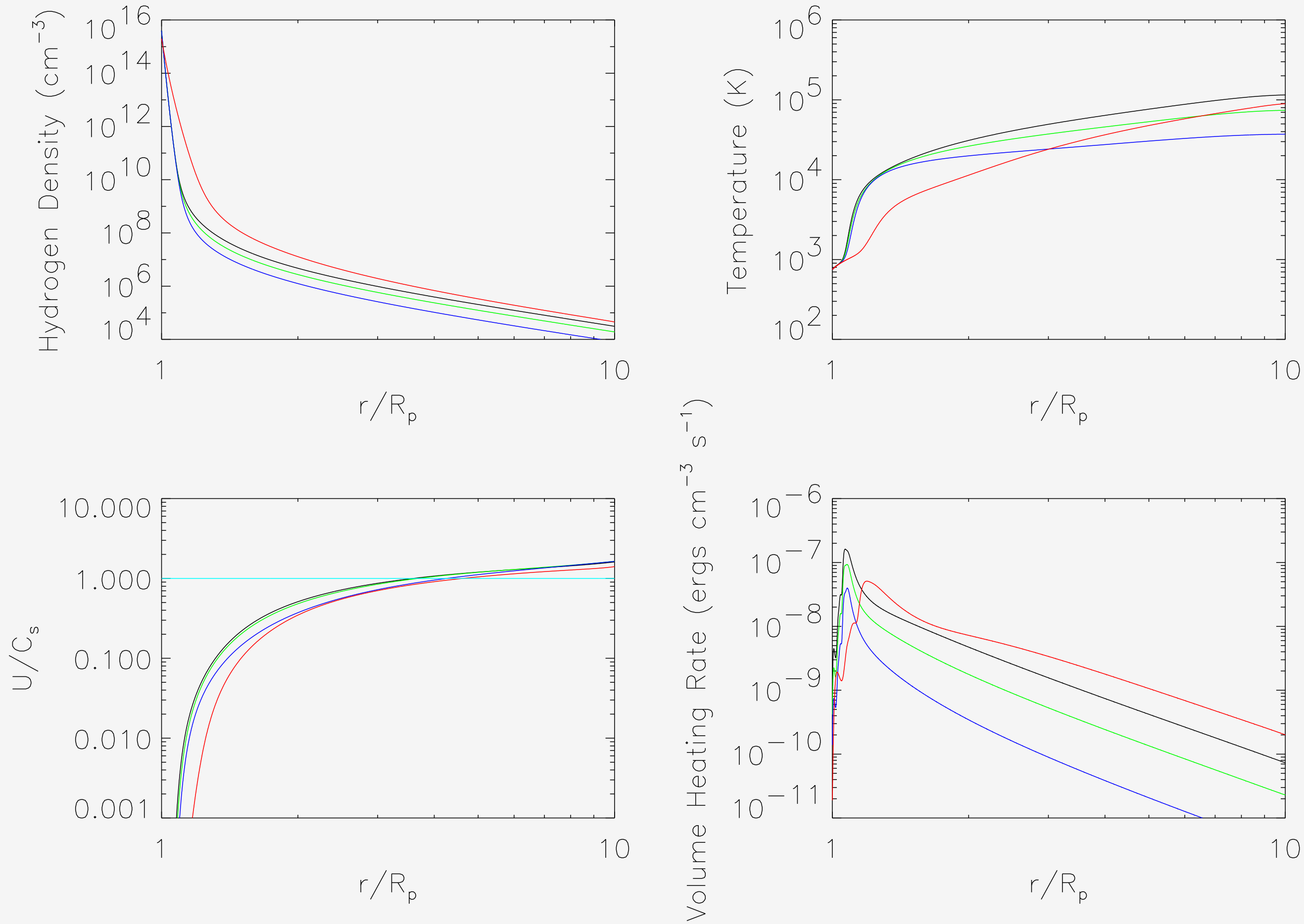
- 104 planetary systems
- 119 planets
- 13 multiple planet systems

- 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