Using Geometric Singular Perturbation Theory to Understand Singular Shocks

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Outline

Conservation Laws and Their Pathologies

- Our focus, in $U_t + F(U)_x \equiv U_t + A(U)U_x = 0$, $\lambda^i(A(U))$ real
  - Dependence of characteristic speeds on state U
  - Example: Burgers equation, $u_t + uu_x = 0$, $\lambda = u$
  - Systems exhibit more complicated dependence(s) than do scalar equations
- Weak solutions are standard
  - Weak form of the system $\int U\phi_t + F(U)\phi_x = 0$
  - Bounded, piecewise smooth solutions exhibit shocks that satisfy Rankine-Hugoniot relation $s[U] = [F(U)]$
- Low-regularity solutions: singular shocks
  - Are not locally bounded
  - Do not satisfy RH relation
  - Satisfy the equation in an even weaker sense (theory by Sever)
  - Some examples can be described by distributions
  - Are best understood by means of approximations

Conservation Law Models for Chromatography

Two components (concentration u_i for chemical i); total mass conserved

$$\frac{\partial}{\partial t}(u_i + v_i(u)) + \frac{\partial}{\partial x} u_i = 0\,, \qquad i = 1, 2$$

- Forced at constant velocity through a column packed with a solid ('fixed bed') onto which they are adsorbed
- Neglect: heat cond., diffusion, viscosity & finite rate of adsorption
- System in thermal and chemical equilibrium
- Amount of chemical i adsorbed is $v_i(u_1, u_2)$
- v_i obtained from adsorption laws (linear rates) $\frac{dv}{dt} = k_1 c(V - v) - k_2 v$
- At equilibrium, $dv/dt = 0$, non-dimensionalized functions are

$$v_i = \frac{a_i u_i}{1 + u_1 + u_2}$$

- Langmuir kinetics: Components compete at different rates, $a_1 < a_2$
- Classical and well-studied system

'Generalized Langmuir' kinetics of Marco Mazzotti, ETH

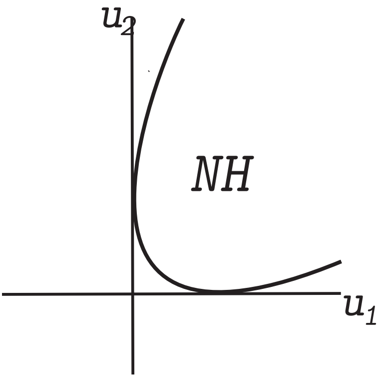
- New model for v:

$$v_i = \frac{a_i u_i}{1 - u_1 + u_2}$$

replaces

$$v_i = \frac{a_i u_i}{1 + u_1 + u_2}$$

- Physically represents 'cooperation' rather than competition for sites

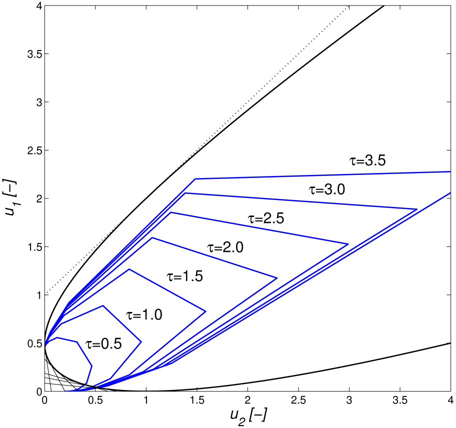


Findings

- System not hyperbolic for some (physically realizable) states
- Restrict to hyperbolic region near 0
- Not all Riemann problems have solutions

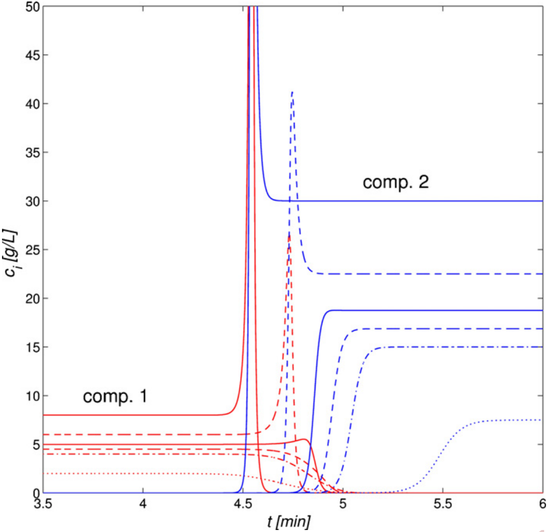
What Happens?

Simulation (phase plane) by Mazzotti



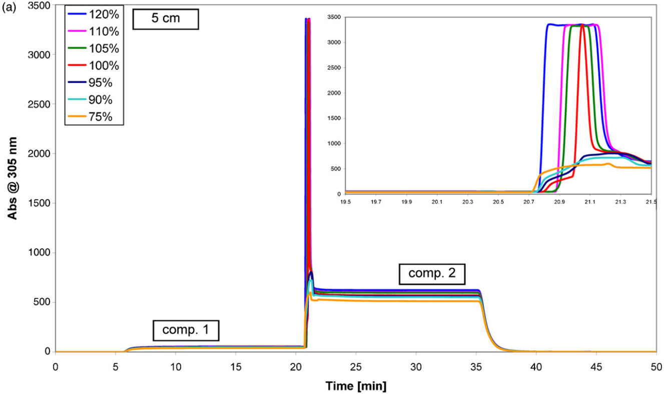
Appearance of Singular Shocks

Simulation (Mazzotti)



Experimental Appearance of Singular Shocks

Experiments (Mazzotti et al)



Components phenetole ($C_8H_{10}O$) and 4-tert-butylphenol ($C_{10}H_{14}O$)
Selected to give (1) cooperation in adsorption rather than competition and (2) linear adsorption rates at experimental concentrations

The Velocity-Entropy System of Isentropic Gas Dynamics

Joint work with Charis Tsikkou, to appear in QAM (following Schecter)

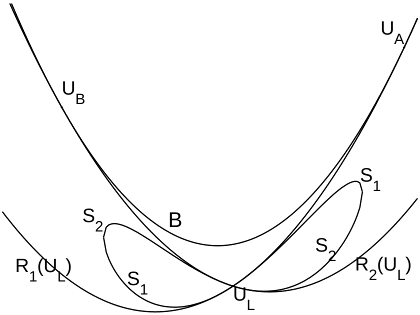
$$\begin{cases} \rho_t + (u_1\rho)_x = 0 \\ (\rho u_1)_t + (\rho u_1^2 + A\rho^\gamma)_x = 0, \end{cases}$$

$$q(\rho) = A\gamma\frac{\rho^{\gamma-1}}{\gamma-1} = \rho^{\gamma-1}$$

$$u_2 = \frac{2-\gamma}{2}u_1^2 - q$$

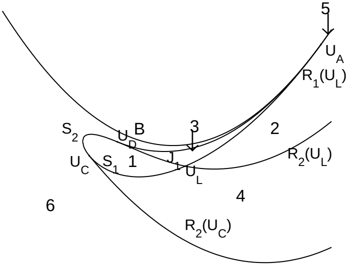
$$1 < \gamma < 5/3$$

$$\begin{cases} u_{1t} + (\frac{(3-\gamma)}{2}u_1^2 - u_2)_x = 0 \\ u_{2t} + [\frac{(2-\gamma)(5-3\gamma)}{6}u_1^3 + (\gamma-1)u_1u_2]_x = 0. \end{cases}$$



- Nonhyperbolic region (above B)
- Compact Hugoniot locus

Region of Classical Riemann Solutions



- Region 1: 1-shock ⇒ 2-shock
- Region 2: 1-rarefaction ⇒ 2-rarefaction
- Region 3: 1-rarefaction ⇒ 2-shock
- Region 4: 1-shock ⇒ 2-rarefaction
- Region 5: 1-rarefaction ⇒ vacuum state ⇒ 2-rarefaction

Approximation by Dafermos Regularization

$$\varepsilon t U_{xx} = U_t + F(U)_x$$

$$\xi = \frac{x}{t}$$

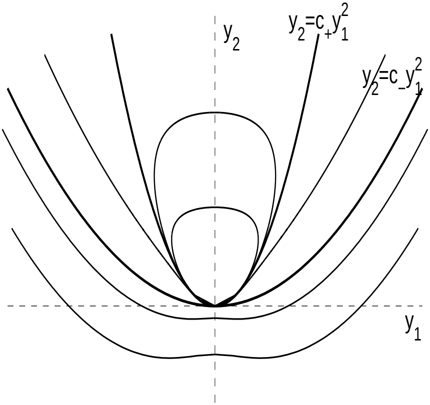
$$\varepsilon \frac{d^2 U}{d\xi^2} = \Big(DF(U) - \xi I \Big) \frac{dU}{d\xi}$$

$$\text{BC } U(-\infty) = U_L\,,\ U(+\infty) = U_R$$

$$U(\xi) = \begin{pmatrix} \frac{1}{\varepsilon^p} y_1\left(\frac{\xi - s}{\varepsilon^q}\right) \\ \\ \frac{1}{\varepsilon^r} y_2\left(\frac{\xi - s}{\varepsilon^q}\right) \end{pmatrix}$$

$$\eta = \tfrac{\xi - s}{\varepsilon^q};\ p = 1,\ q = 2 = r;$$

$$\frac{dY}{d\eta} = F(Y)$$



Inner part/Outer part

Existence of Profiles via Geometric Singular Perturbation Theory: Krupa, Szmolyan & Schecter

GSPT answers questions:

- How is the singular part of the solution (the homoclinic orbit) connected to the outer part (constant states)?
- What happens to the RH relation?
- What is limiting process $\varepsilon \to 0$?

$$U_t + F(U)_x = \varepsilon t U_{xx}$$

Self-similar $\xi = \frac{x}{t}$

$$\begin{aligned} \varepsilon U'' &= -\xi U' + F(U)' \\ &= (-\xi U)' + U + F(U)' \end{aligned}$$

Define

$$W \equiv F(U) - \xi U - \varepsilon U'$$

then $W' = -U$ and system is

$$\begin{aligned} \varepsilon U' &= F(U) - \xi U - W \\ W' &= -U \\ \xi' &= 1 \end{aligned}$$

Example of a fast-slow system

$$\begin{aligned} \varepsilon x' &= f(x, y, \varepsilon) \\ y' &= g(x, y, \varepsilon) \end{aligned}$$

The Idea

Fast time $\tau = \theta/\varepsilon$

System $\begin{cases} \varepsilon x' &= f(x, y, \varepsilon) \\ y' &= g(x, y, \varepsilon) \end{cases}$

1. Solve in slow time
   $\varepsilon = 0 \begin{cases} 0 &= f(x, y, 0) \\ y' &= g(x, y, 0) \end{cases}$
2. Solve in fast time
   $\varepsilon = 0 \begin{cases} \dot{x} &= f(x, y, 0) \\ \dot{y} &= 0 \end{cases}$
3. Show that these singular orbits are connected if $\varepsilon > 0$
4. To use 'Fenichel Theory', which requires *normally hyperbolic* invariant manifolds (orbits), 'blow up' some orbits if necessary

Our system uses τ:

$$\dot{U} = F(U) - \xi U - W$$
$$\dot{W} = -\varepsilon U$$
$$\dot{\xi} = \varepsilon$$

with invariant sets

$$\{W = F(U) - \xi U\}$$

and scaling with $\eta = \tau/\varepsilon$ and $Y = \mathrm{diag}\{\varepsilon, \varepsilon^2\} U$:

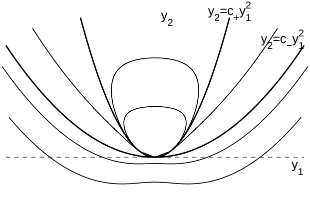
$$Y' = F(Y)$$
$$W' = -\mathrm{diag}\{0, 1\} Y$$
$$\xi' = 0$$

Reduced System

Blow up of eq'm $E = \{Y = 0, \varepsilon = 0\}$

$$Y = \mathrm{diag}(\bar{r}, \bar{r}^2)\overline{Y},\ \varepsilon = \bar{r}\bar{\varepsilon}$$

$$|\overline{Y}|^2 + \bar{\varepsilon}^2 = 1$$



Outer system $U \to \infty$ in finite time

Inner system $Y \Rightarrow$ homoclinic orbit

$$[W] = \begin{cases} 0 \\ \int y_2 \end{cases}$$

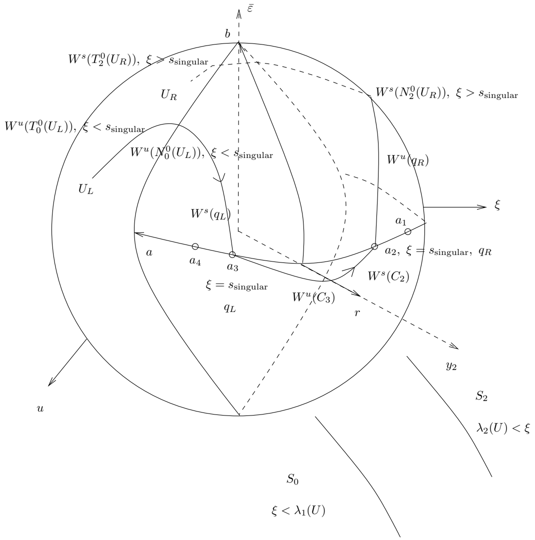
so one RH cond holds, not both

Coord chart on blown up surface:

$$\begin{cases} a = \frac{\bar{y}_1}{\sqrt{\bar{y}_2}} = \frac{y_1}{\sqrt{y_2}} = \frac{u_1}{\sqrt{u_2}} \\ r^2 = \bar{r}^2\bar{y}_2 = y_2 = \varepsilon^2 u_2 \\ b = \frac{\bar{\varepsilon}}{\sqrt{\bar{y}_2}} = \frac{\varepsilon}{\sqrt{y_2}} = \frac{1}{\sqrt{u_2}} \end{cases}$$

$$\begin{aligned} a' =&(2-\gamma)a^2 - 1 - \tfrac{(2-\gamma)(5-3\gamma)}{12}a^4 \\ &+\tfrac{b}{2}\big(-\xi a - 2bw_1 + b^2 a w_2\big) \\ r' =&\tfrac{r}{6}\Big(\tfrac{(2-\gamma)(5-3\gamma)}{2}a^3 - 3b\xi \\ &+3(\gamma-1)a - 3b^3 w_2\Big) \\ w_1' =& -rab, \quad w_2' = -r, \quad \xi' = rb^2 \\ b' =& -\tfrac{b}{6}\Big(\tfrac{(2-\gamma)(5-3\gamma)}{2}a^3 - 3b\xi \\ &+3(\gamma-1)a - 3b^3 w_2\Big) \end{aligned}$$

Overview of the Singular Trajectories



a_3 & a_2: equilibria of $\{a, b, r\}$ system

Verify

- normal hyperbolicity
- transversality
- hypotheses of corner lemma
- role of strict overcompressibility

The Result

Theorem

In the velocity-entropy system with $1 < \gamma < 5/3$, assume that U_R is in the interior of region 7 with respect to U_L, so that with

$$s_{singular}(U_L, U_R) \equiv \frac{F_1(U_L) - F_2(U_R)}{u_{L1} - u_{R1}},$$

we have

$$0 < F_2(U_L) - F_2(U_R) - s_{singular}(u_{L2} - u_{R2}),$$

and the strict inequalities

1. $s_{singular}(U_L, U_R) < \lambda_1(U_L)$
2. $\lambda_2(U_R) < s_{singular}(U_L, U_R)$

hold. Then there exists a singular shock connecting U_L and U_R; that is, a solution U_ε of the Dafermos regularization which becomes unbounded as $\varepsilon \to 0$.

Summary

- Original model problem (isothermal gas dynamics, $\gamma = 1$) led to discovery of weak solutions of very low regularity (measures)
- Theory developed by Sever for systems with this structure
- Sever's theory is based on distributions (δ-functions)
- GSPT, developed by Fenichel, Kopell, Kaper, Jones, Krupa, Szmolyan, and others, provides insight into structure of singular solutions (more detail than distributions)
- Other approaches given by generalized distribution theory of Colombeau et al
- Recent model from chromatography has physical significance, and cannot be analysed via classical distributions
- Analysis of chromatography system using GSPT is in progress (with Ting-Hao Hsu, Martin Krupa, and Charis Tsikkou)