Continuum Models of Two Phase Flow in Porous Media

Michael Shearer

North Carolina State University
Department of Mathematics

Research supported by NSF grants DMS 0968258 FRG, DMS 0636590 RTG

Acknowledgements

- Students and former students

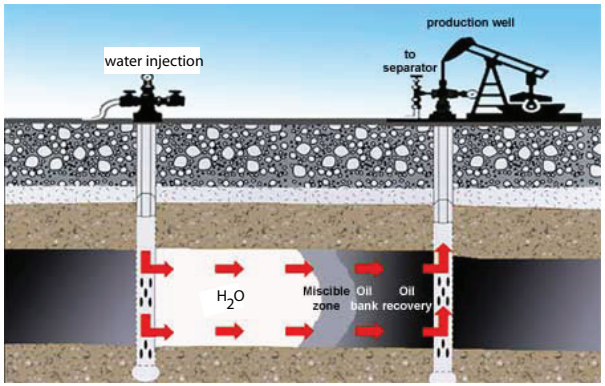
  Rachel Levy (Harvey Mudd College)
  Kim Spayd (Gettysburg College)
  Melissa Strait (NC State University)

- Collaborators

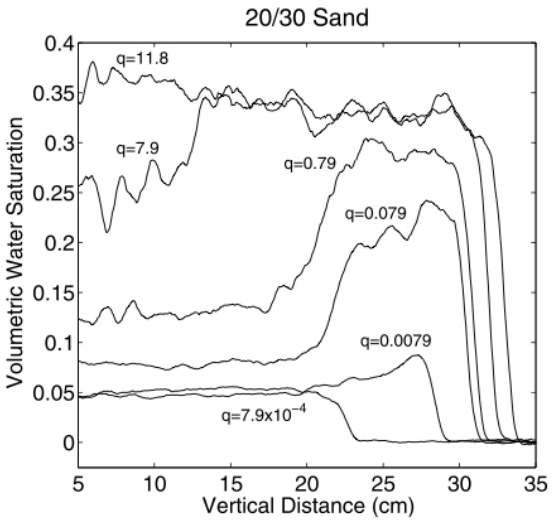
  Ruben Juanes, Luis Cueto-Felgueroso (MIT Engineering)
  Zhenzheng Hu (NC State University)

Applications

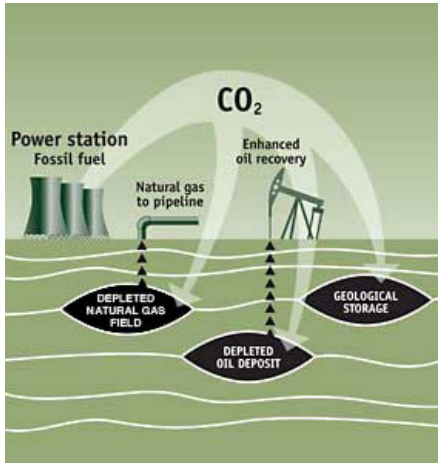
Oil recovery: water flood

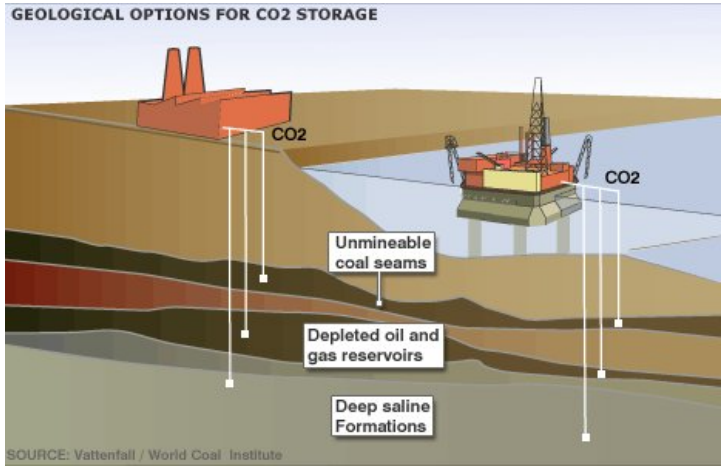


Water infiltration under gravity (DiCarlo 2004)



Carbon Sequestration in Deep Saline Aquifers





Introduction I

- Framework: Conservation of mass; Darcy's law; incompressibility
- Buckley-Leverett flux $f(u)$ (1942) u is saturation
  non-convex conservation law $u_t + f(u)_x = 0$
- Modeling: pressure difference p^c across interfaces: interfacial energy
- Classical approach: $p^c = p^e(u)$ equilibrium pressure; decreasing in u
  $$u_t + f(u)_x = -(H(u)p^e(u)_x)_x$$
- Dynamic effects: Hassanizadeh and Gray (1991,1993):
  $p^c = p^e(u) - \tau u_t$

  Netherlands group: undercompressive shocks; sharp shocks

  Pop, van Duijn, Peletier, Cuesta, Fan (2006-2012)

Introduction II

- 2-d stability/instability for Lax shocks: hyperbolic/elliptic system
- Phase field modeling: Juanes (2008), Witelski (1998), based on polymer mixtures: introduce stored energy function with capillary effects

  Capillary tube gas/liquid finger: degenerate fourth order PDE

  Dynamical systems trick for traveling waves
- Carbon sequestration: Huppert, Neufeld, Hesse, ... (2008-2011). Discontinuous dependence in conservation law to allow for deposition of CO_2 bubbles as plume propagates in brine (deep saline aquifer)

  Track interface; non-standard wave interactions

2-D Model

$u(x, y, t)$: **saturation** (vol. fraction) of water, $(1 - u)$: oil saturation
$p(x, y, t)$: **pressure** in water

<u>*Conservation of mass*</u> with Darcy's law: velocity $\mathbf{v} = -\lambda(u)\nabla p$:

$$\boxed{\phi \frac{\partial u}{\partial t} - \nabla \cdot (\lambda(u)\nabla p) = 0} \qquad \phi = \text{porosity}, \ \lambda(u) = \frac{Kk(u)}{\mu}$$

K = absolute permeability, $k(u)$ = relative permeability, μ = viscosity

<u>*Incompressibility:*</u> $\nabla \cdot \mathbf{v}^{\mathbf{Total}} = 0$

$$\boxed{\nabla \cdot \Big(\Lambda(u)\nabla p + \lambda^{oil}(u)\nabla p^c(u)\Big) = 0}$$

$\Lambda = \lambda^{water} + \lambda^{oil}, \quad p^c = p^{oil} - p$: capillary pressure;

For simplicity, neglect gravity, set $\phi = 1$.

One-Dimensional Equation for $u(x,t)$: $u_t - (\lambda p_x)_x = 0$

$$\nabla \cdot \mathbf{v}^{\mathbf{Total}} = 0 \quad \Longrightarrow \quad \mathbf{v}^{\mathbf{Total}} = (v^T, 0) \; = \; \text{constant, after rescaling } t$$

Thus,
$$\Lambda p_x + (\Lambda - \lambda) p_x^c = -v^T$$

Eliminate p_x :
$$p_x = -\frac{v_T}{\Lambda(u)} - \left(1 - \frac{\lambda(u)}{\Lambda(u)}\right) p_x^c$$

Then
$$\boxed{u_t + f(u)_x = -\left(H(u) p_x^c\right)_x}$$

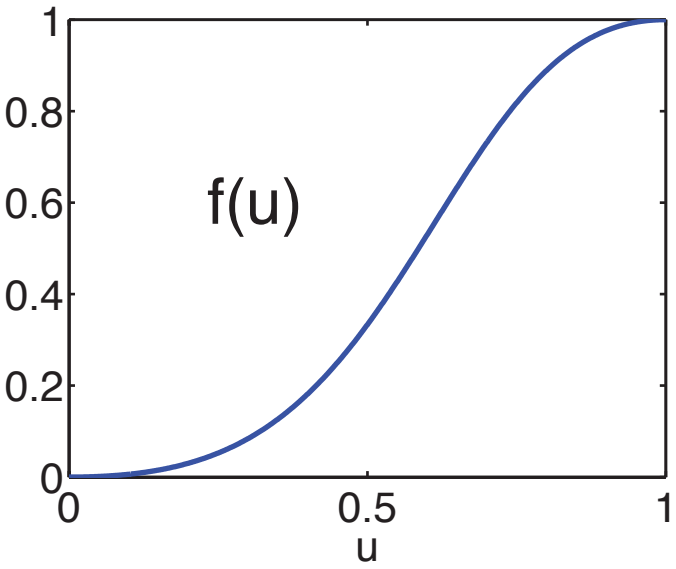
$$f(u) = v^T \frac{\lambda(u)}{\Lambda(u)}, \qquad H(u) = \frac{\lambda(u)}{\Lambda(u)} \left(\Lambda(u) - \lambda(u)\right)$$

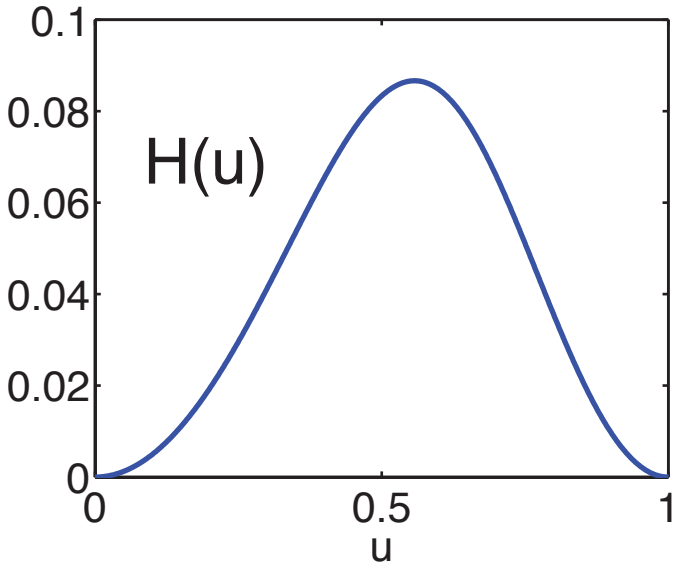
$$\boxed{u_t + f(u)_x = -\left(H(u)p_x^c\right)_x}$$

$$f(u) = v^T \frac{\lambda(u)}{\Lambda(u)}, \qquad H(u) = \frac{\lambda(u)}{\Lambda(u)}\left(\Lambda(u) - \lambda(u)\right)$$

Fractional flow rate Dissipation coefficient

Recall: $\Lambda(u)$ is total mobility: $\Lambda(u) - \lambda(u) = \lambda^{oil}(1-u)$
λ, λ^{oil} are positive, increasing convex functions, with $\lambda(0) = \lambda^{oil}(0) = 0$.





$u_t + f(u)_x = -\left(H(u)p_x^c\right)_x$, but what to do about p^c?

- Buckley-Leverett (1942): *ignore it:* $p^c = 0$

  scalar non-convex conservation law $u_t + f(u)_x = 0$

  Lax-Oleinik construction: *rarefaction-shock interface*

- Classical approach: equilibrium capillary pressure depends on saturation: $p^c = p^e(u)$, a decreasing function: $\frac{d}{du}p^e(u) < 0$.

  The PDE is parabolic but degenerate at $u = 0, 1$.

  Max principle: $0 \leq u \leq 1$ is positively invariant.

  Lax-Oleinik solutions replaced by smooth approximation.

- Hassanizadeh and Gray (1991, 1993): rate dependence in p^c :

$$p^c = p^e(u) - \tau u_t$$

- Modified Buckley-Leverett equation

$$u_t + f(u)_x = -\left(H(u)\frac{\partial}{\partial x}p^e(u)\right)_x + \tau\left(H(u)u_{tx}\right)_x$$

- Equation is dissipative-dispersive. No maximum principle, but positive invariance of $0 \leq u \leq 1$ (Yabin Fan thesis 2012)
- Analogous equation: modified BBM-Burgers:

$$u_t + (u^3)_x = \alpha u_{xx} - \beta u_{xxt}$$

Traveling waves for undercompressive shocks (Spayd thesis, 2012)

- Explicit construction similar to modified KdV-Burgers:

$$u_t + (u^3)_x = \alpha u_{xx} - \beta u_{xxx}$$

(Jacobs, McKinney, Shearer, 1995; LeFloch book, 2002)

Traveling Wave Solutions

$$u(\xi) = u(x - st) \Rightarrow \quad -su' + (f(u))' = [H(u)u']' - s\tau\,[H(u)u'']'$$

Integrating with boundary conditions $u(\pm\infty) = u_\pm$ leads to second order ODE: $-s(u - u_-) + f(u) - f(u_-) = H(u)u' - s\tau H(u)u''$

Rescale $u = u(\frac{x-st}{\sqrt{s\tau}})$ and write as first order system of ODEs:

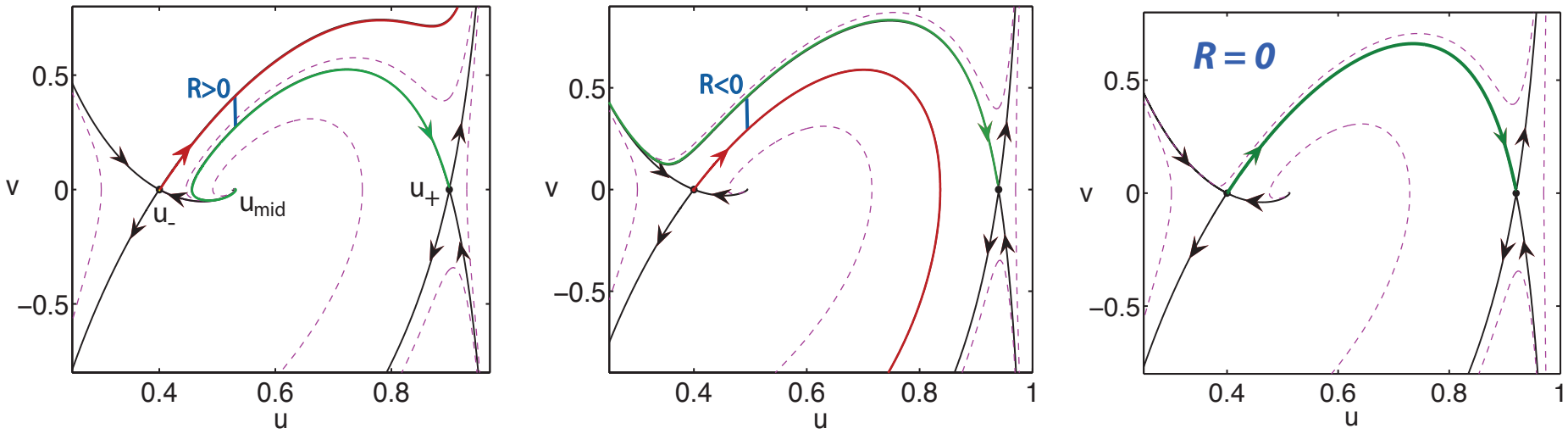
$$\boxed{\begin{aligned} u' &= v \\ v' &= \frac{1}{\sqrt{s\tau}}v + \frac{1}{H(u)}\left[s(u - u_-) - f(u) + f(u_-)\right] \end{aligned}}$$

Singular at $u = 0,\ u = 1$, where $H(u) = 0$

Saddle-Saddle Connections

Phase portraits of ODE system: up to three equilibria
$(u_e, 0)$: $(u_\pm, 0), (u_{\text{mid}}, 0)$, $s = (f(u_e) - f(u_-))/(u_e - u_-)$

Analyze phase plane with separation function $R(u_-, u_+, \tau)$



Saddle-saddle connection: $R = 0$:
heteroclinic orbit from $(u_-, 0)$ to $(u_+, 0)$ *undercompressive shock*

Numerical procedure

For $\tau < \infty$, fix u_- and determine $u_+ = u_\Sigma(u_-)$ for which $R(u_-, u_+, \tau) = 0$

Monotonicity of $u_\Sigma(u_-)$ from Melnikov integral: derivatives of R

For $\tau = \infty$, determine (u_-, u_Σ) by using exact integral:

$$\frac{1}{2}\frac{d}{du}v^2 = \frac{1}{H(u)}\left[s(u-u_-) - f(u) + f(u_-)\right] \equiv G(u; u_-, u_+)$$

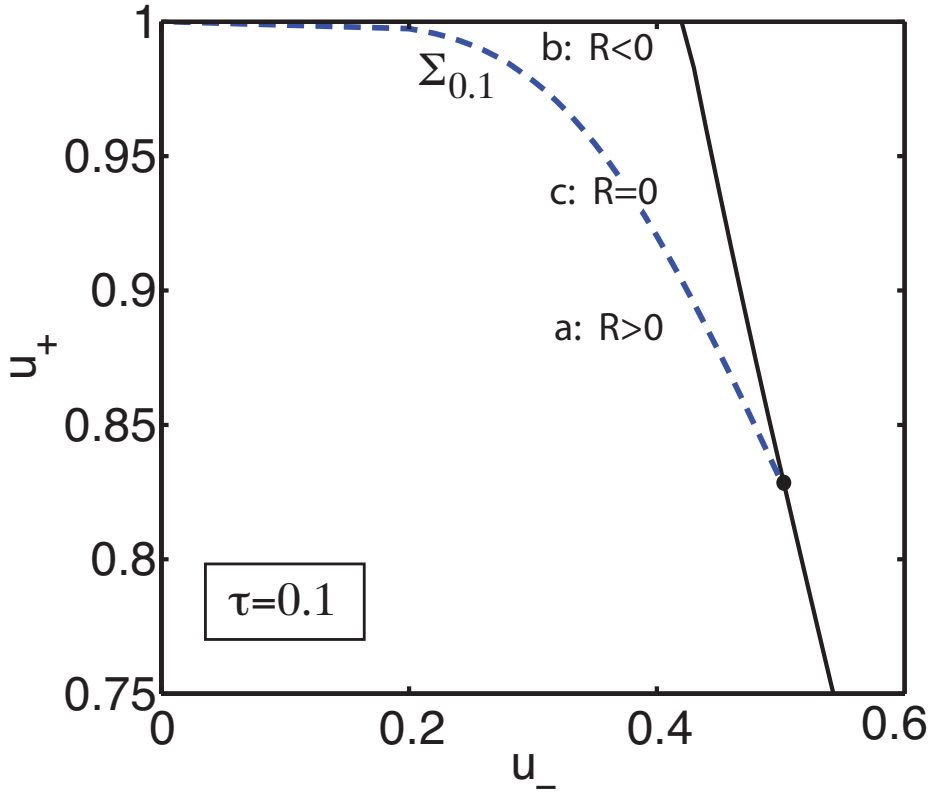
Thus: connection when $\boxed{\int_{u_-}^{u_+} G(u; u_-, u_+)\, du = 0 : \quad u_+ = u_\Sigma(u_-)}$

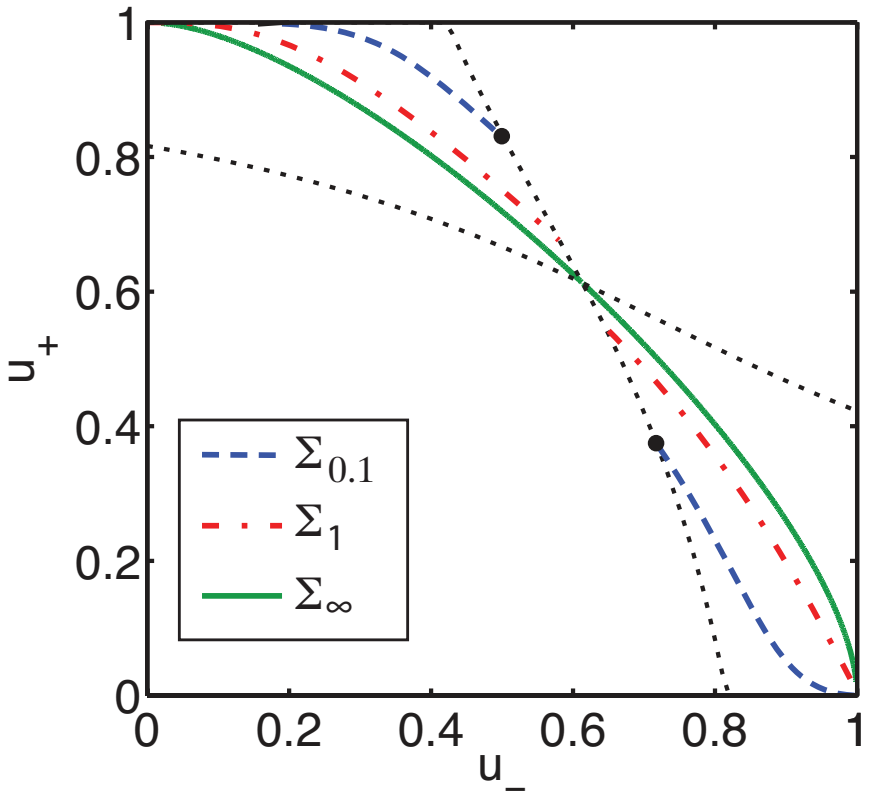
Asymptotics in corners: e.g., $u_- \to 0,\ u_+ \to 1$:

$$u_+ = u_\Sigma(u_-) \sim 1 - u_-^M$$

Σ_τ Curves

Fix $\tau > 0$, plot (u_-, u_+) with saddle-saddle connection $u_- \to u_+$





Scalar conservation law: $u_t + f(u)_x = 0$

Idealization: no capillary pressure; characteristic speed $f'(u)$

Scale invariant solutions: building blocks for solving initial value problem

Rarefactions

$$u(x,t) = \begin{cases} u_- & \text{if } x < f'(u_-)t \\ r(\frac{x}{t}) & \text{if } f'(u_-)t \le x \le f'(u_+)t \\ u_+ & \text{if } x > f'(u_+)t \end{cases}$$

Shocks

$$u(x,t) = \begin{cases} u_- & \text{if } x < st \\ u_+ & \text{if } x > st \end{cases}$$

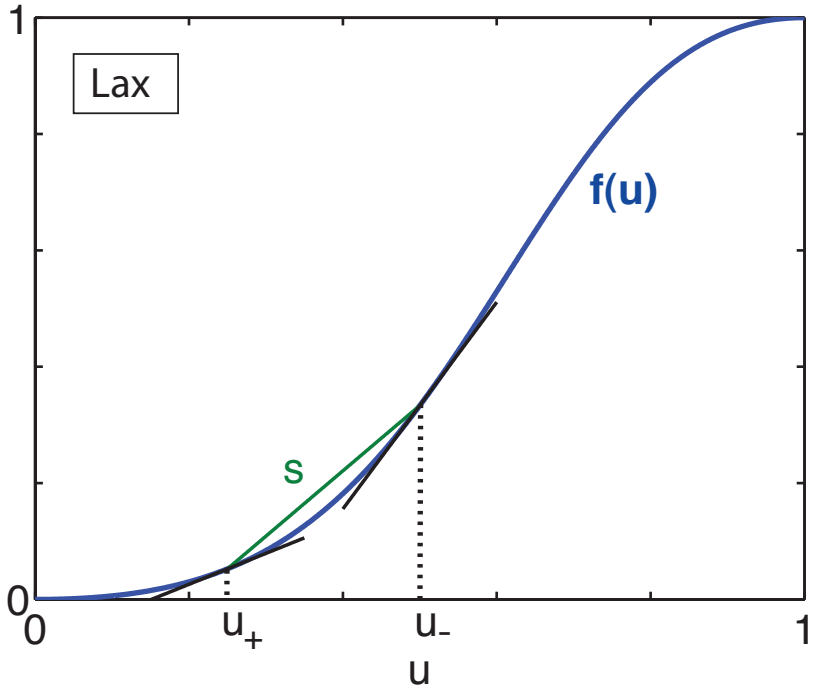
Rankine-Hugoniot condition: shock speed $s = \dfrac{f(u_+) - f(u_-)}{u_+ - u_-}$

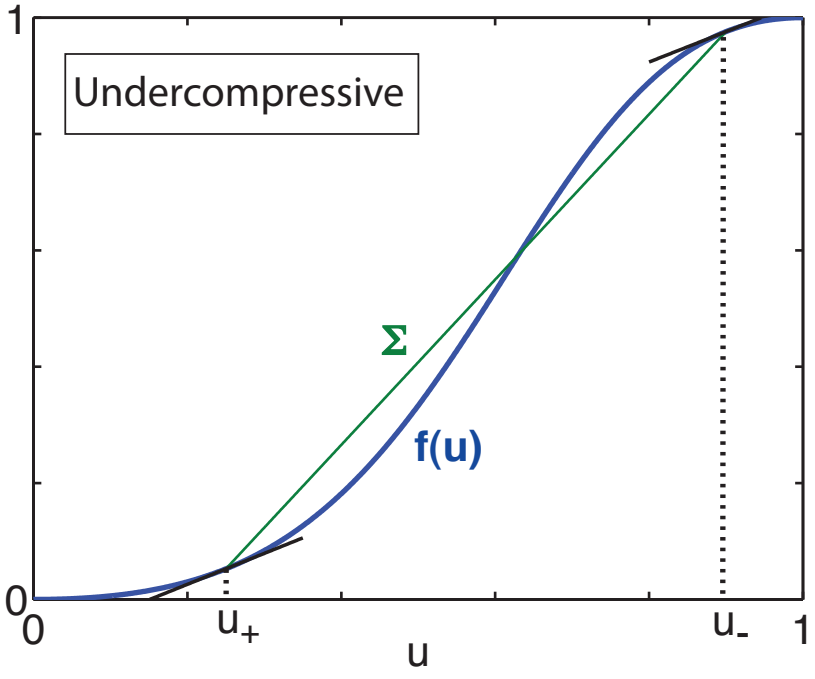
Admissible Shocks

$f'(u_+) < s < f'(u_-)$ $\boxed{Lax}$ shock is admissible if there is a traveling wave from $u_- = u_{mid}$ (unstable node) to u_+ (saddle point)

$s > f'(u_\pm)$ **PLUS:** shock has corresponding traveling wave: $\boxed{undercompressive}$ shock Σ.

Jacobs, McKinney, Shearer (1995), LeFloch Book (2002)

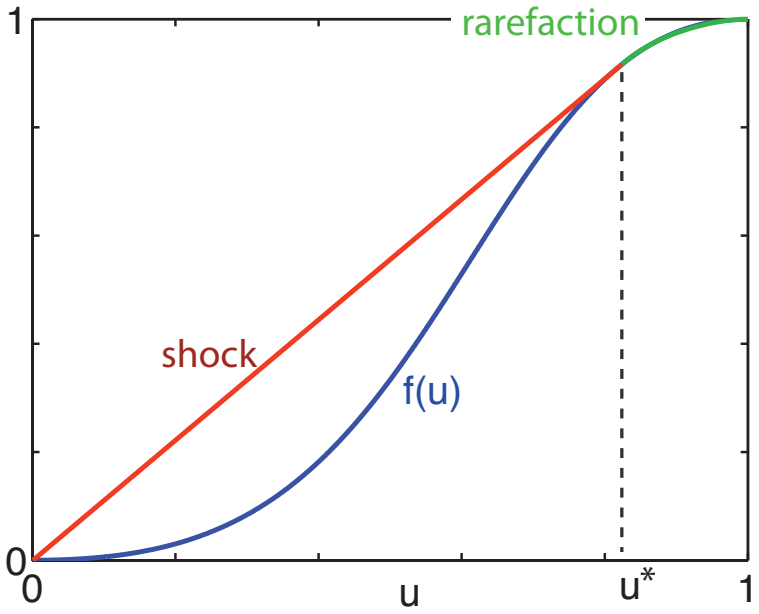




Buckley-Leverett solution 1942

Solve conservation law with initial jump from all water $u_- = 1$ to all oil $u_+ = 0$: water flooding:

$$u_t + f(u)_x = 0, \qquad u(x,0) = \begin{cases} 1 & \text{if } x < 0 \\ 0 & \text{if } x > 0 \end{cases}$$

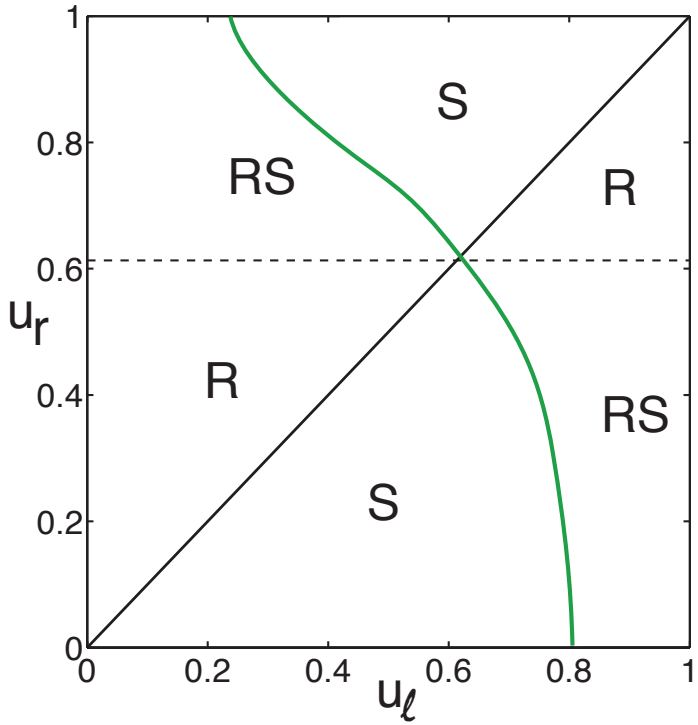


Solution: rarefaction from $u_- = 1$ to u^*; Lax shock from u^* to $u_+ = 0$: *rarefaction-shock.*

The Riemann Problem: Classical Solution

Solve conservation law with initial jump from u_ℓ to u_r

$$u_t + f(u)_x = 0, \qquad u(x,0) = \begin{cases} u_\ell & \text{if } x < 0 \\ u_r & \text{if } x > 0 \end{cases}$$

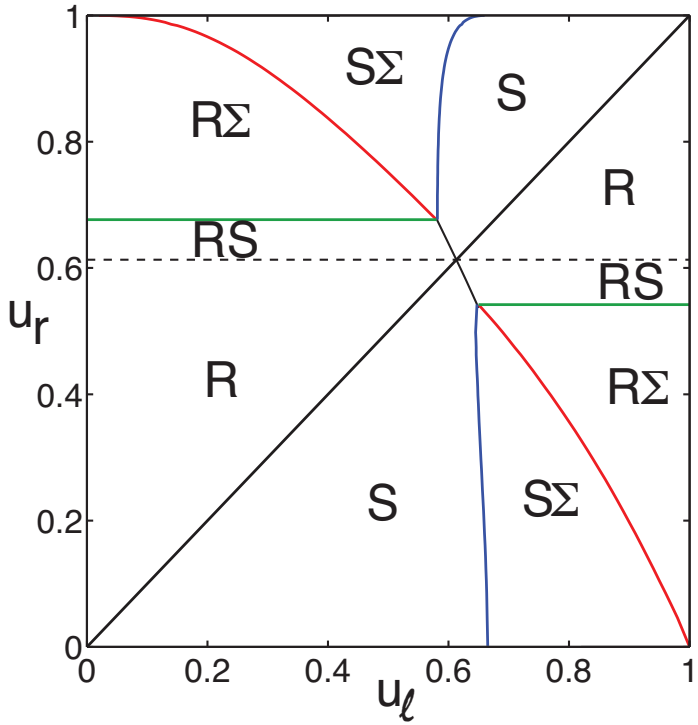


R: Rarefaction Wave
S: Lax Shock
RS : Rarefaction - Shock

The Riemann Problem; dynamic capillary pressure

$$(RP): \quad u_t + f(u)_x = 0, \qquad u(x,0) = \begin{cases} u_\ell & \text{if } x < 0 \\ u_r & \text{if } x > 0 \end{cases}$$

Solutions of (RP): leading order approximations to solutions of modified Buckley-Leverett equation



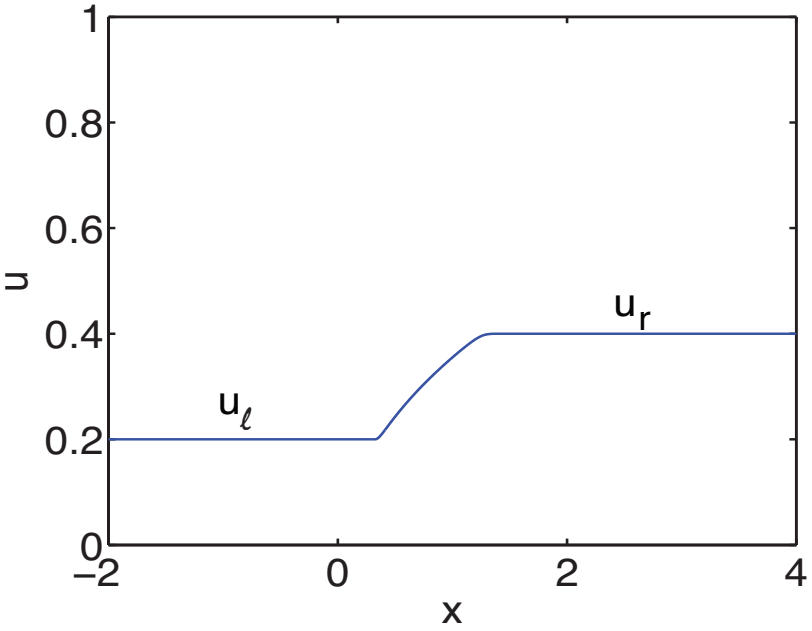
R: Rarefaction Wave
S: Admissible Lax Shock
Σ : Undercompressive Shock

For every $(u_\ell, u_r) \in (0,1)$, there is a solution that stays in $(0,1)$ even though $S\Sigma$ solutions are nonmonotonic.

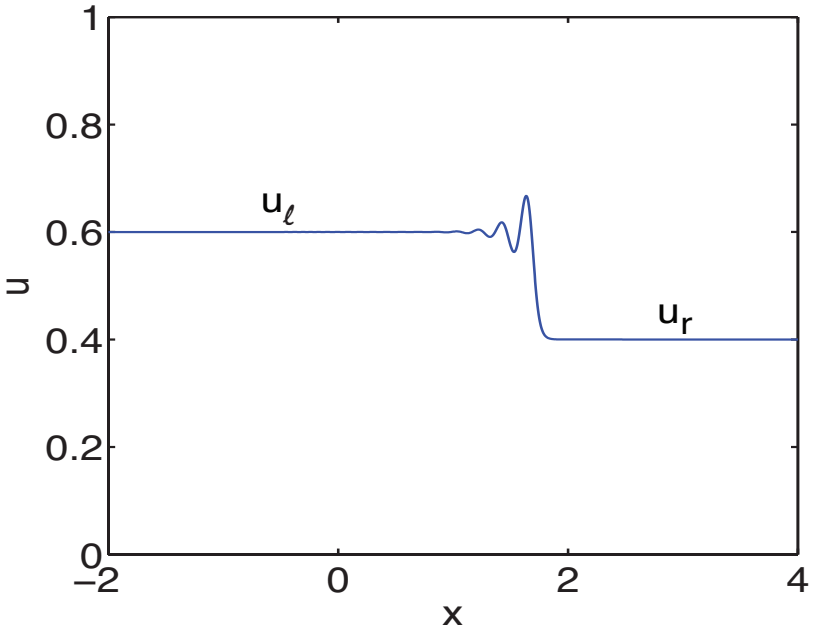
PDE Simulations

Full PDE: $\boxed{u_t + f(u)_x = (H(u)u_x)_x + \tau\,(H(u)u_{tx})_x}$

$u_\ell \in (0, u_r)$: *rarefaction wave*

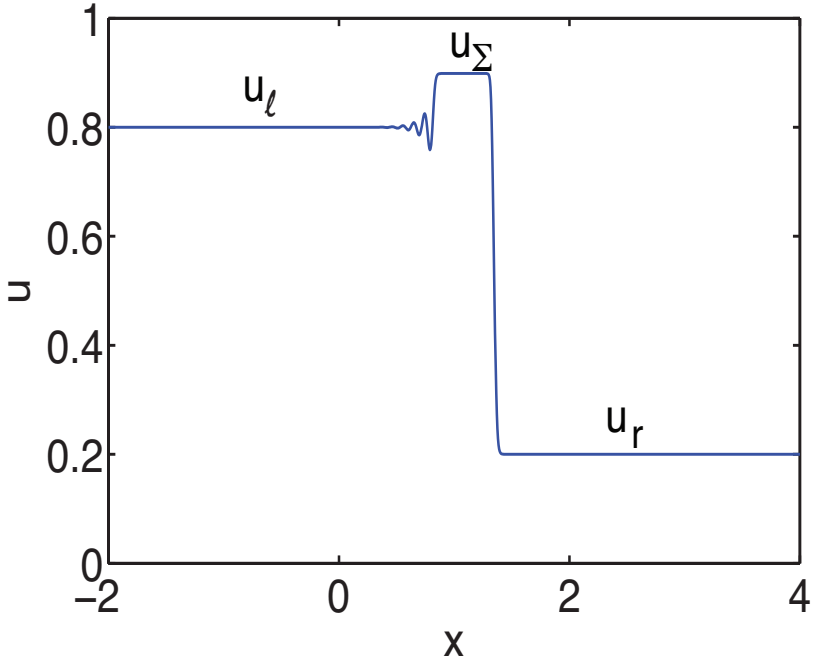


$u_\ell \in (u_r, u_{mid})$: *Lax shock*

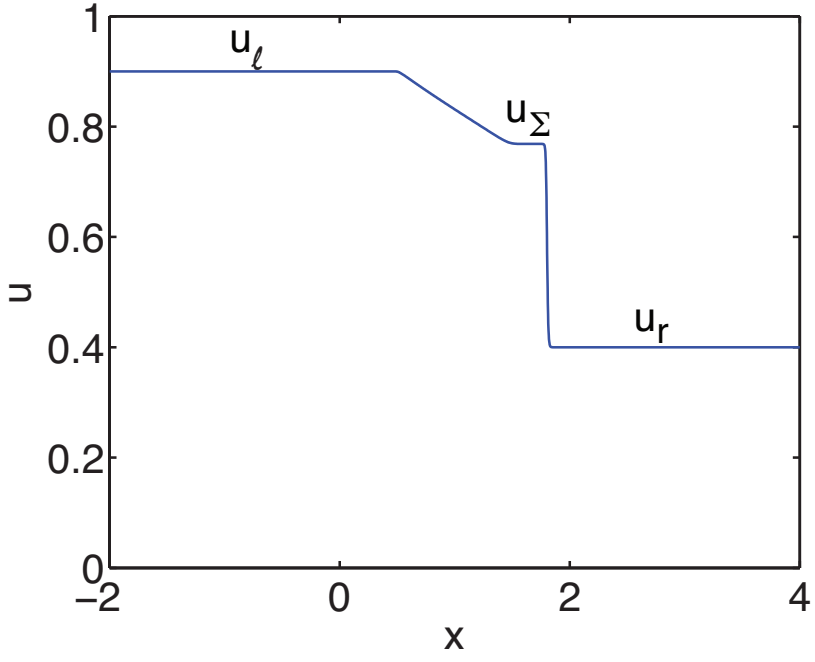


PDE Simulations - Nonclassical Solutions

$u_\ell \in (u_{mid}, u_\Sigma)$:
Lax shock u_ℓ to u_Σ
undercompressive shock
u_Σ to u_r



$u_\ell \in (u_\Sigma, 1)$:
rarefaction wave u_ℓ to u_Σ
undercompressive shock
u_Σ to u_r



‘Sharp’ Traveling waves TW $u = u(x - st)$

$$u_t + f(u)_x = -\left(H(u)\frac{\partial}{\partial x}p^e(u)\right)_x + \tau\left(H(u)u_{tx}\right)_x$$

$$-s(u - u_-) + f(u) - f(u_-) = -H(u)p^e(u)' - s\tau H(u)u'', \quad u(\pm\infty) = u_\pm$$

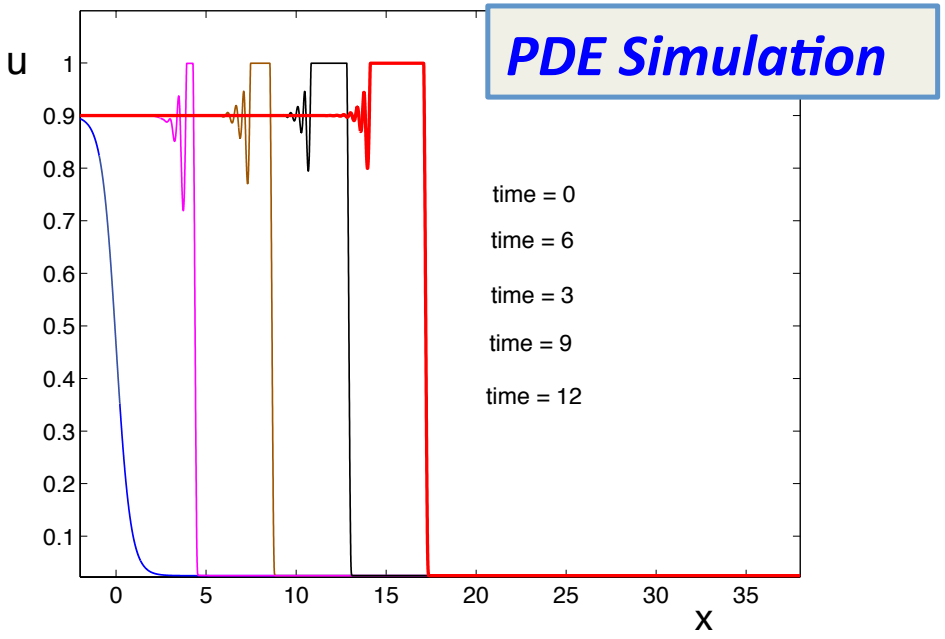
after one integration

Singular at $u = 0, 1$ Can have connections up to $u = 1$, or down to $u = 0$ depending on relative permeability functions at $u = 0, 1$

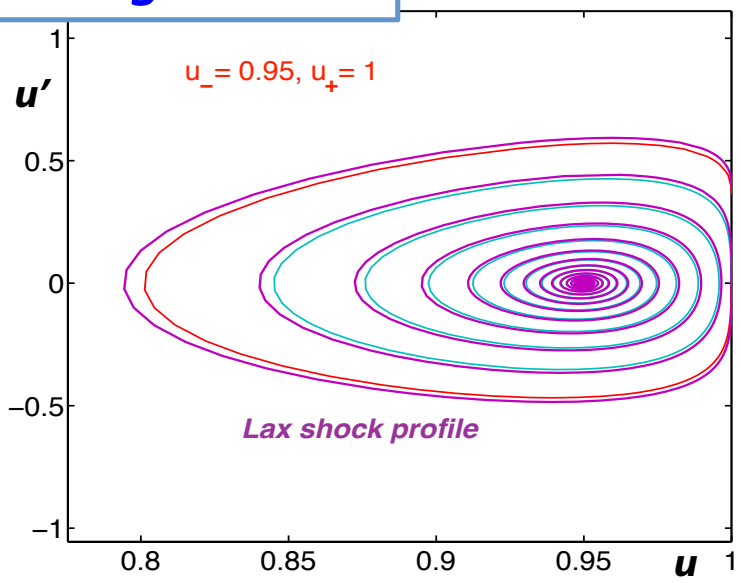
Example: $\lambda(u) = u^{3/2}$; $\lambda^{oil}(u) = (1 - u)^{3/2}$

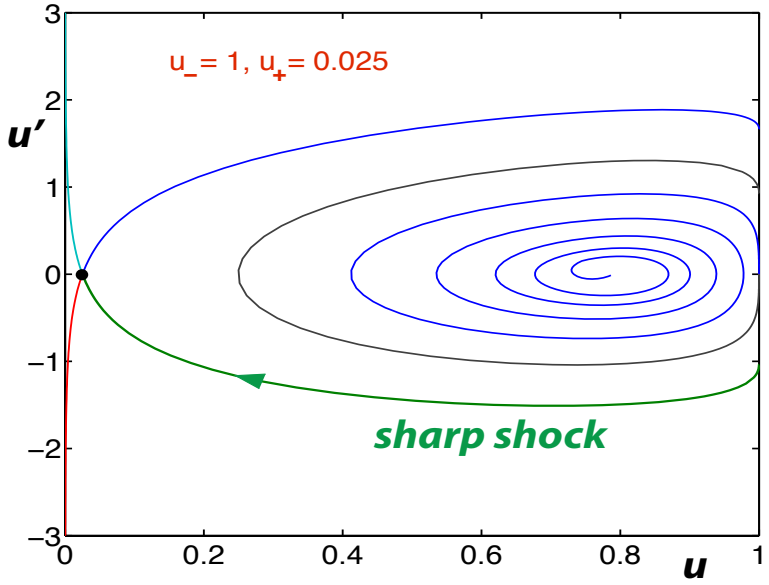
Pop, Cuesta, van Duijn (2011): *sharp shock* TW with corner at $u = 1$

Relative permeabilities
Integrable case:
$K(u) = u^{3/2}$



Phase Portraits:
Traveling waves



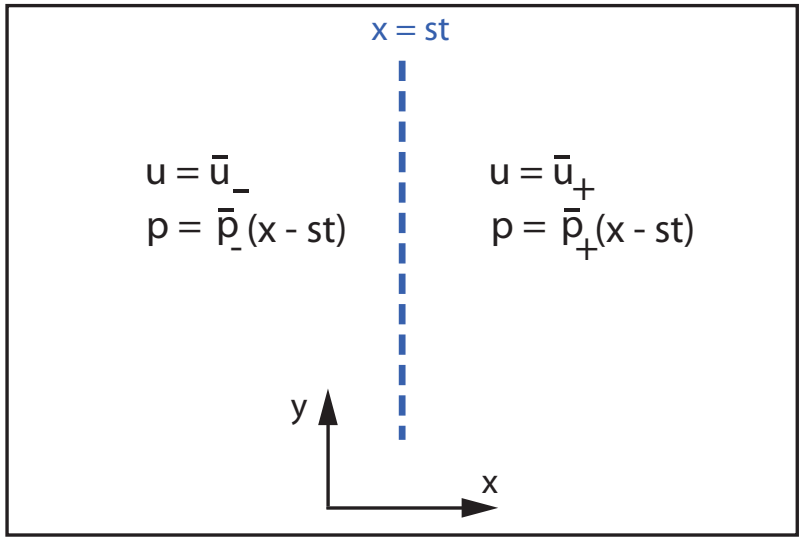


Planar Lax shock $u_t + f(u)_x = 0$

Interface $\bar{x} = st$; velocity $v_\pm = -\lambda_\pm \partial_x p_\pm$; mobility $\lambda_\pm = Kk(\bar{u}_\pm)/\mu$

Continuous pressure $p = \bar{p}_\pm(x - st) = -\frac{v_\pm}{\lambda_\pm} z = -\frac{v^T}{\Lambda_\pm} z, \quad z = x - st;$

shock location: $\bar{z} = \bar{x} - st = 0$



Shock speed

$$s = \frac{f(\bar{u}_+) - f(\bar{u}_-)}{\bar{u}_+ - \bar{u}_-}$$

Lax condition:

$f'(\bar{u}_+) < s < f'(\bar{u}_-)$

Characteristic speeds $f'(\bar{u}_\pm)$

2-dimensional linearized stability of Lax shocks

2-d equations with $p_c \equiv 0$ variables u, p saturation, pressure:

$$\begin{aligned} \frac{\partial u}{\partial t} - \nabla \cdot (\lambda(u) \nabla p) &= 0 \\ \nabla \cdot (\Lambda(u) \nabla p) &= 0 \end{aligned} \tag{1}$$

Interface $x = \hat{x}(y, t)$, normal in t, x, y : $(-\hat{x}_t, 1, -\hat{x}_y)$
Jump condition at shock: $([q] = q_+ - q_-)$

$$\begin{aligned} -\hat{x}_t [u] - [\lambda(u) p_x] + \hat{x}_y [\lambda(u) p_y] &= 0 \\ -[\Lambda(u) p_x] + \hat{x}_y [\Lambda(u) p_y] &= 0 \end{aligned} \tag{2}$$

Base shock: $u = \bar{u}_\pm, p = \bar{p}_\pm(x - st), \hat{x} = st$, constants $\bar{u}_\pm, \bar{p}_\pm, V$

$$s = \frac{f(\bar{u}_+) - f(\bar{u}_-)}{\bar{u}_+ - \bar{u}_-}, \quad f(u) = v^T \frac{\lambda(u)}{\Lambda(u)}, \quad \bar{p}_\pm = -\frac{v^T}{\Lambda(\bar{u}_\pm)}$$

Equations $\frac{\partial u}{\partial t} - \nabla \cdot (\lambda(u)\nabla p) = 0,\ \nabla \cdot (\Lambda(u)\nabla p) = 0$

$$\begin{aligned} \frac{\partial u}{\partial t} - \lambda'(u)\nabla u \cdot \nabla p - \lambda(u)\Delta p &= 0 \\ \Lambda'(u)\nabla u.\nabla p + \Lambda(u)\Delta p &= 0 \end{aligned} \tag{1}$$

Linearize about shock on each side:
$u = \bar{u} + U(x, y, t), p = \bar{p}(x - st) + P(x, y, t)$

$$\begin{aligned} U_t - \lambda'(\bar{u})\bar{p}U_x - \lambda(\bar{u})\Delta P &= 0 \\ \Lambda'(\bar{u})\bar{p}U_x + \Lambda(\bar{u})\Delta P &= 0 \end{aligned} \tag{2}$$

Thus, $\Delta P = -\frac{\Lambda'(\bar{u})}{\Lambda(\bar{u})}\bar{p}U_x.$ Subs. into U_t equation:

$$U_t - \bar{p}\left(\lambda'(\bar{u}) - \lambda(\bar{u})\frac{\Lambda'(\bar{u})}{\Lambda(\bar{u})}\right)U_x = 0$$

CLAIM: Lax shock $\implies$ U has to be zero.

$$U_t - \bar{p}\left(\lambda'(\bar{u}) - \lambda(\bar{u})\frac{\Lambda'(\bar{u})}{\Lambda(\bar{u})}\right)U_x = 0, \quad \bar{u} = \bar{u}_\pm$$

Let $U(x,y,t) = w(x-st)e^{i\alpha y}e^{\sigma t}$. Then, with $z = x - st$, $w' = \frac{dw}{dz}$:

$$\sigma w - sw' - \bar{p}\,\lambda(\bar{u})\left(\frac{\lambda'(\bar{u})}{\lambda(\bar{u})} - \frac{\Lambda'(\bar{u})}{\Lambda(\bar{u})}\right)w' = 0$$

But $f(u) = v^T\lambda(u)/\Lambda(u)$, $\bar{p}\,\lambda(\bar{u}) = -f(\bar{u})$ so we have

$$\sigma w = (s - f'(\bar{u}))\,w', \quad \text{with solutions } w(z) = a_\pm e^{\beta_\pm z},$$

$$\sigma = \beta_\pm(s - f'(\bar{u}_\pm))$$

For a Lax shock, $f'(\bar{u}_+) < s < f'(\bar{u}_-)$.
Thus, $Re\ \sigma \geq 0$ implies $w(z)$ does not decay at $z = \pm\infty$ unless $w \equiv 0$.
Consequently, $\boxed{U \equiv 0}$

2-d stability: perturb pressure in linearized equations

$$u = \bar{u}_\pm; \quad p = \bar{p}_\pm z + P; \quad P(z, y, t) = q_\pm(z) e^{i\alpha y + \sigma t}$$

$$\hat{z} = \hat{x} - Vt = a e^{i\alpha y + \sigma t}, \quad z = x - \hat{x}$$

We seek $\sigma = \sigma_1 \alpha,\ \alpha > 0.$ Linearized equations: $\Delta P = 0$:

$$q''_\pm - \alpha^2 q_\pm = 0 \tag{1}$$

Decaying solutions: $q_\pm = b_\pm e^{\mp \alpha z}, \ \pm z > 0,$

Next: linearize jump conditions: two equations for three coefficients

$$a, b_-, b_+$$

Linearized jump conditions (no perturbation on u)

$$\sigma a[\bar{u}] + [\lambda(\bar{u})q'] = 0 \tag{1}$$

$$[\Lambda(\bar{u})q'] = 0 \tag{2}$$

Equation (2):

$$\boxed{\Lambda(\bar{u}_+)b_+ = -\Lambda(\bar{u}_-)b_-} \tag{3}$$

Then (1) implies

$$b_-\Lambda(\bar{u}_-)(f(\bar{u}_+) - f(\bar{u}_-)) = -\frac{\sigma}{\alpha}a(\bar{u}_+ - \bar{u}_-)v^T$$

But $(f(\bar{u}_+) - f(\bar{u}_-))/(\bar{u}_+ - \bar{u}_-) = s$, the shock speed, so

$$\boxed{b_-\Lambda(\bar{u}_-)s = -a\frac{\sigma}{\alpha}v^T} \tag{4}$$

2-dimensional stability: third equation for $a, b_\pm$

Third equation comes from continuity of pressure (linearized) at $z = \hat{z}(y,t) = ae^{i\alpha y + \sigma t}$

$$p = \bar{p}_\pm z + q_\pm(z)e^{i\alpha y + \sigma t}, q_\pm = b_\pm e^{\mp \alpha z} \quad (\pm z > 0)$$

Consequently,

$$\boxed{\bar{p}_+ a + b_+ = \bar{p}_- a + b_-} \tag{5}$$

Thus, $\quad (\bar{p}_+ - \bar{p}_-)a = -\frac{\sigma}{\alpha}\frac{v^T}{s}a\left(\frac{1}{\Lambda(\bar{u}_+)} + \frac{1}{\Lambda(\bar{u}_-)}\right), \quad$ (from (3,4))

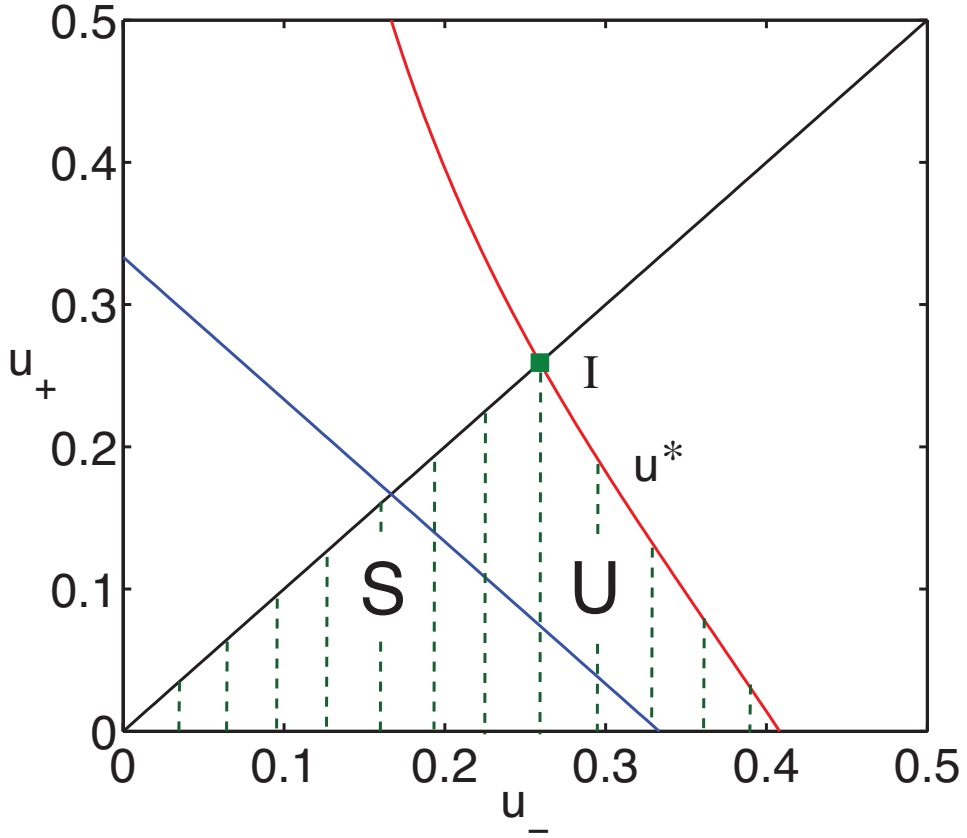
Since $\bar{p}_\pm = -\frac{v^T}{\Lambda(\bar{u}_\pm)}$, we obtain, for $a \neq 0$:

$$\boxed{\frac{\sigma}{\alpha} = s\frac{\Lambda(\bar{u}_-) - \Lambda(\bar{u}_+)}{\Lambda(\bar{u}_-) + \Lambda(\bar{u}_+)}}$$

Interpretation of stability condition: quadratic relative permeabilities: $k(u) = \kappa u^2$

Lax shocks for $u_+ < u_- \leq u^*$, $\quad f'(u^*) = (f(u_+) - f(u^*))/(u_+ - u^*)$

Stability boundary: $u_+ = -u_- + \frac{2M}{M+1}$



$M = 0.2 \quad \dfrac{2M}{M+1} = \dfrac{1}{3}$

Inflection point **I** of $f(u)$ at $u_I = 0.2591$

S: Stable Lax shocks

U: Unstable Lax shocks

Fingering Instability - Zhengzheng's Simulations

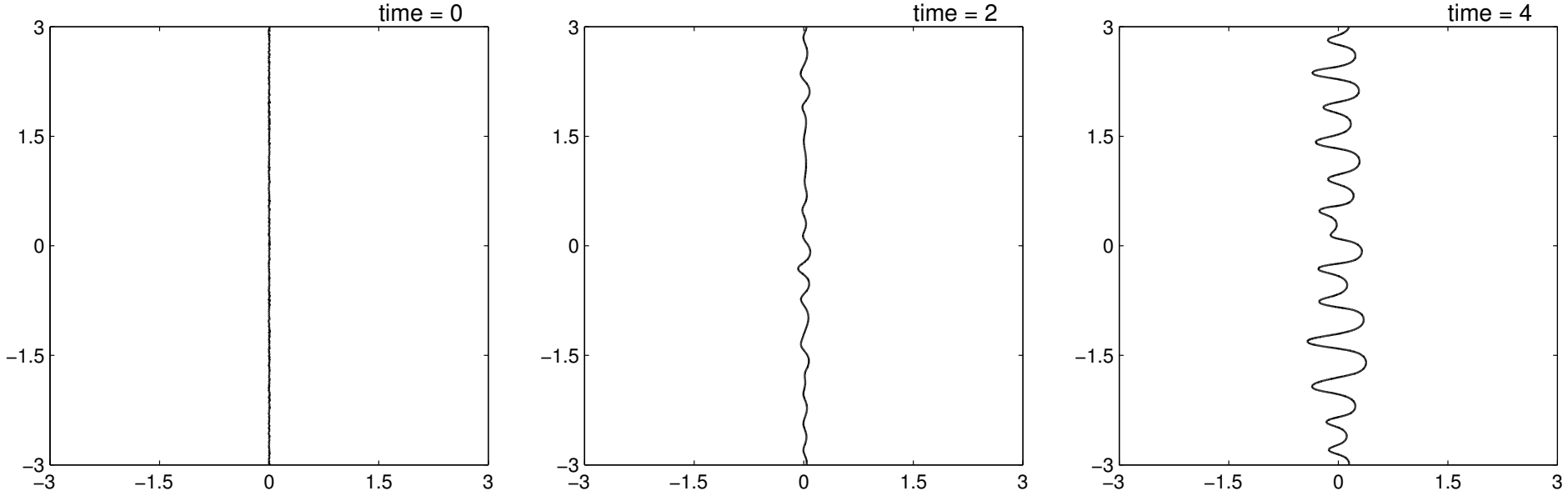
Full parabolic/elliptic system with capillary pressure $p^c = -u + \tau u_t$

Crank-Nicolson time-step; upwind advection; periodic side boundary conditions, moving frame, plot middle contour $u = \frac{1}{2}(u_- + u_+)$

$\Delta t = O(10^{-3})$, $\Delta x = \Delta y = O(10^{-2})$

Initial condition: $u =$ randomly perturbed hyperbolic tangent

$u_- = 0.2, u_+ = 0, M = 0.05$



Numerical Simulations - Stable case

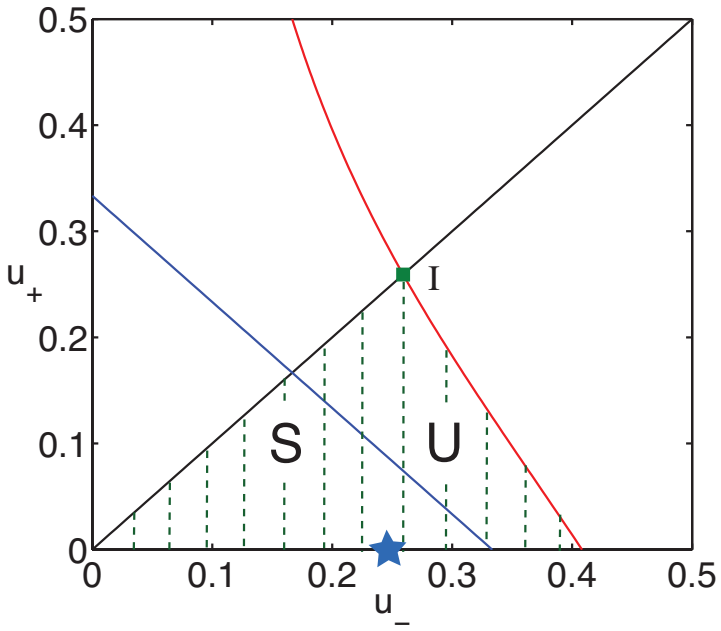
$M = 0.2$

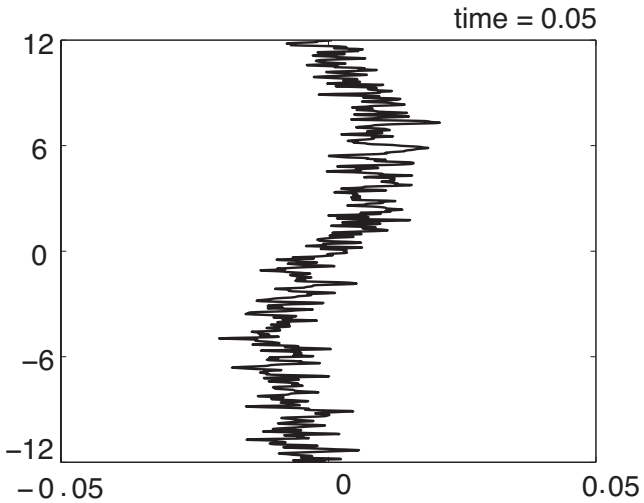
$u_- = 0.25, u_+ = 0$

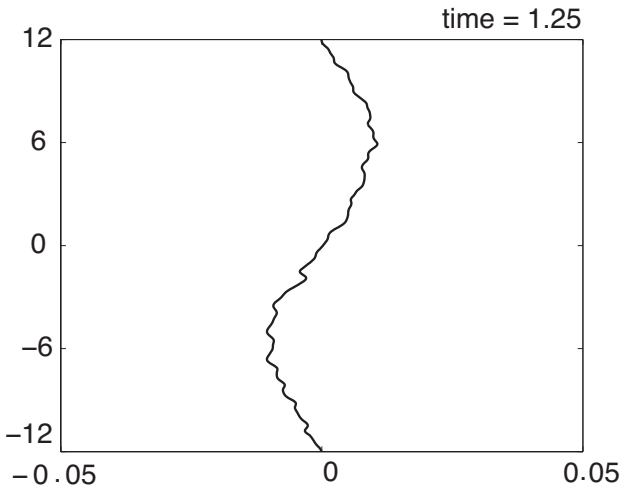
Oil-water mixture displaces oil

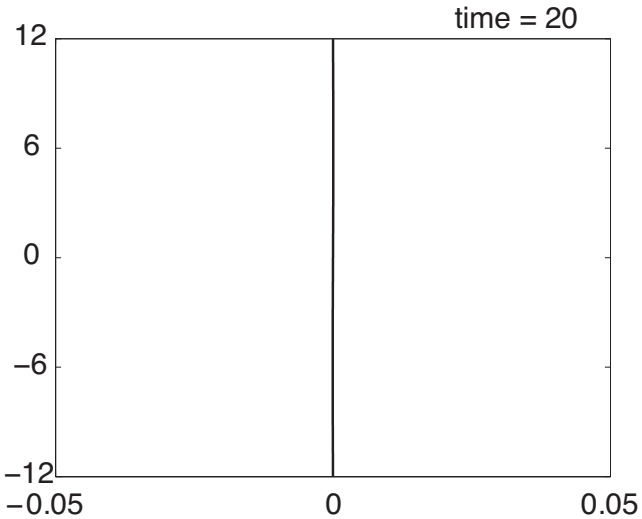
Initial perturbation decays

Zoomed-in contour









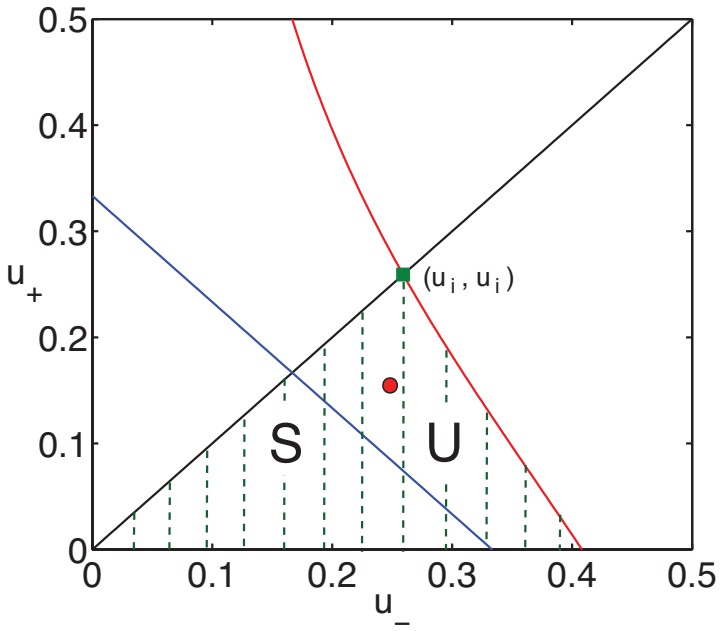
Numerical Simulations: Unstable case: Fingering Instability

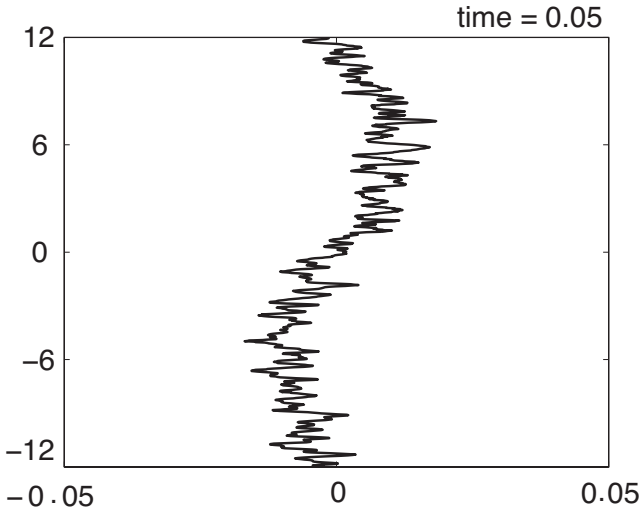
$M = 0.2$

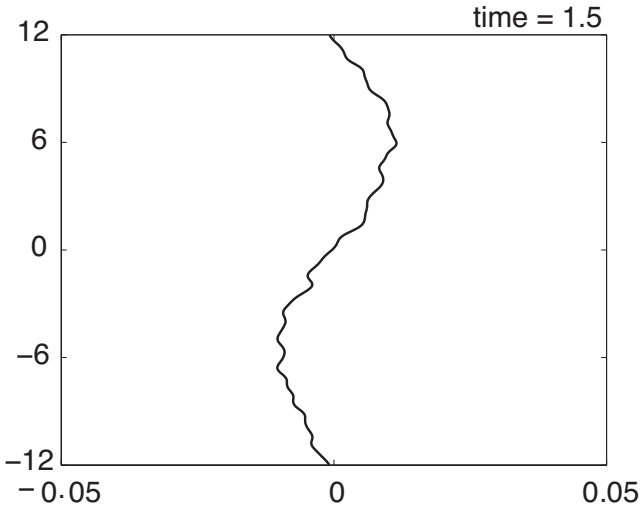
$u_- = 0.25, u_+ = 0.15$

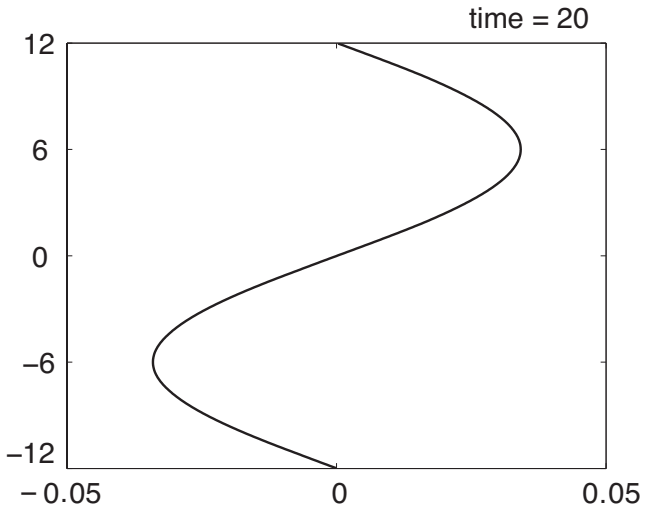
weak Lax shock

Initial perturbation grows $\Rightarrow$ fingering instability









Conclusions: stability/fingering instability in 2-d

Analysis of hyperbolic/elliptic system linearized around 1-d shock
Linear dependence of growth rate σ on transverse wave number α distinguishes stable waves from unstable

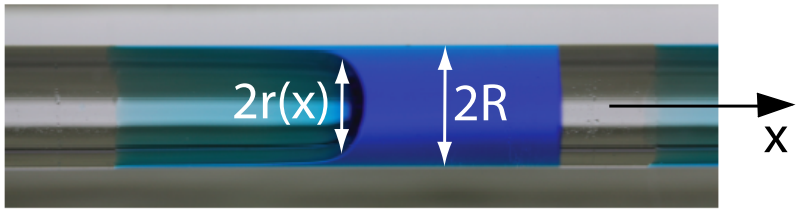
Numerical simulations of full parabolic/elliptic system confirm results; (Riaz and Tchelepi (2006) also conducted numerical experiments)

Weak Lax shocks may be stable or unstable

Oil/water mixture displacing oil can be stable.

K. Spayd, M. Shearer and Z. Hu, Applicable Analysis, 2012.

Back to basics: capillary pressure in a capillary tube



$\gamma = 1/Ca = \sigma/U\eta$

$Ca =$: capillary number

balance between surface tension σ and viscosity η.

Saturation u : area fraction

$u(x,t) = r(x)^2/R^2$.

Write equation in form

$$u_t + f(u)_x = -\gamma\partial_x\left[f(u)\lambda(u)\partial_x\psi\right]$$

$f(u) = u/(u + (1-u)^3)$

Fractional flow rate for air/water (Bear 1972)

$\lambda(u) = (1-u)^3$

$\psi = \frac{\delta F}{\delta u}$, F : free energy

$F = F^0(u) + \kappa(u)F^1(u_x)$

F^0 : bulk free energy

$F^1(u_x)$: interfacial energy

$\kappa(u)$: interfacial energy weight

Phase field model: $F = F^0(u) + \kappa(u)F^1(u_x)$

Cueto-Felgueroso and Juanes, PRL (2008, 2011)

Simple choices:

$$\boxed{F^0(u) = -\frac{\Sigma}{R}(1-u)^2u^2 + 2\frac{\gamma_{wg}\cos\theta}{R}(1-u)^2}$$

Double-well potential; tangent construction (like equal area rule)

$\Sigma = \gamma_{sw} - \gamma_{sg} - \gamma_{wg} < 0$ spreading parameter

θ : static contact angle Young-Laplace law at contact line
$\gamma_{sw} - \gamma_{sg} = \gamma_{wg}\cos\theta$, set $\gamma = \gamma_{wg}$

$$\boxed{F^1(u_x) = \Gamma u_x^2}$$

$\Gamma = C(\theta)\gamma R$

Phase field model: $u_t + f(u)_x = -\gamma\partial_x\left[f(u)\lambda(u)\partial_x\psi\right]$

Variational derivative: $\psi = \frac{\delta F}{\delta u}$

$$\psi = -C_1 u(1-u)(1-2u) + C_2\sqrt{\kappa(u)}\partial_x(\sqrt{\kappa(u)}\partial_x u), \quad C_1 > 0, C_2 > 0$$

Chemical potential for polymer mixture:

de Gennes: J. Chem. Phys. (1980); Witelski, Appl. Math. Lett. (1998)

Benzi, Sbragaglia, Bernachi, Succi: *Binary fluid mixtures,* PRL (2011)

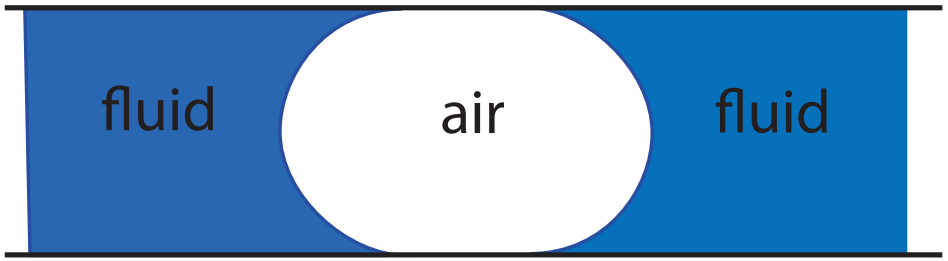
$$\boxed{\partial_t u + \partial_x f(u) = \gamma\partial_x\left[H(u)Q(u)\partial_x u\right] - \gamma\partial_x\left[H(u)\partial_x C_2\sqrt{\kappa(u)}\partial_x(\sqrt{\kappa(u)}\partial_x u)\right]}$$

$$Q(u) = C_1(6u^2 - 6u + 1), \quad H(u) = f(u)\lambda(u)$$

Cahn-Hilliard type equation

Static solutions: bubbles and compactons

Now choose $\kappa(u)$ so that a static bubble is an equilibrium solution



static air bubble

Ends of bubble are spherical caps (take contact angle $\theta = 0,$ or π) :

$$u(x) = r^2 = 1 - x^2,\ 0 \le x \le 1. \text{ Thus } u' = -2x = -2\sqrt{1-u},\ u'' = -2.$$

Here, tube radius $R = 1,\quad \theta = \pi,\quad {}' = \partial_x$

$$\partial_x \left[f(u)\lambda(u)\partial_x \psi \right] = 0$$

Consequently,

$$f(u)\lambda(u)\psi' = c_0 = 0, \quad \text{since } f(0) = 0$$

$$\psi(u) = -C_1 G(u) + C_2\sqrt{\kappa}\partial_x(\sqrt{\kappa}\partial_x u)); \quad G(u) = u(1-u)(1-2u)$$

$$f(u)\lambda(u)\psi' = 0 \implies \psi = c_1 = 0, \quad \text{since } \kappa(0) = 0$$

Thus,

$$m(u)(m(u)u')' = Ku(1-u)(1-2u), \qquad K = C_2/C_1, m(u) = \sqrt{\kappa(u)}.$$

$u(x) = 1 - x^2 \implies x = \sqrt{1-u}$: ODE for $m(u)$:

$$m(u)\left(\frac{dm}{du}4(1-u) - 2m(u)\right) = KG(u) = Ku(1-u)(1-2u).$$

But $\kappa(u) = m(u)^2$. Then

$$\frac{d\kappa}{du}(1-u) - \kappa = \frac{K}{2}u(1-u)(1-2u).$$

LHS $= \frac{d}{du}((1-u)\kappa)$, so $(1-u)\kappa = \frac{K}{2}(\frac{1}{2}u^2 - u^3 + \frac{1}{2}u^4)$. That is,

$$\boxed{\kappa(u) = \frac{K}{4}(1-u)u^2}$$

General contact angles θ : Coeff. of interfacial energy κ

Similar result for general contact angle $\theta,\ 0 < \theta < \pi$:

$$u = \sec^2\theta - x^2/R^2$$

$$\kappa(u) = \frac{K(\theta)u^2(1-u)^2}{4(\sec^2\theta - u)}, \quad 0 \le u \le 1.$$

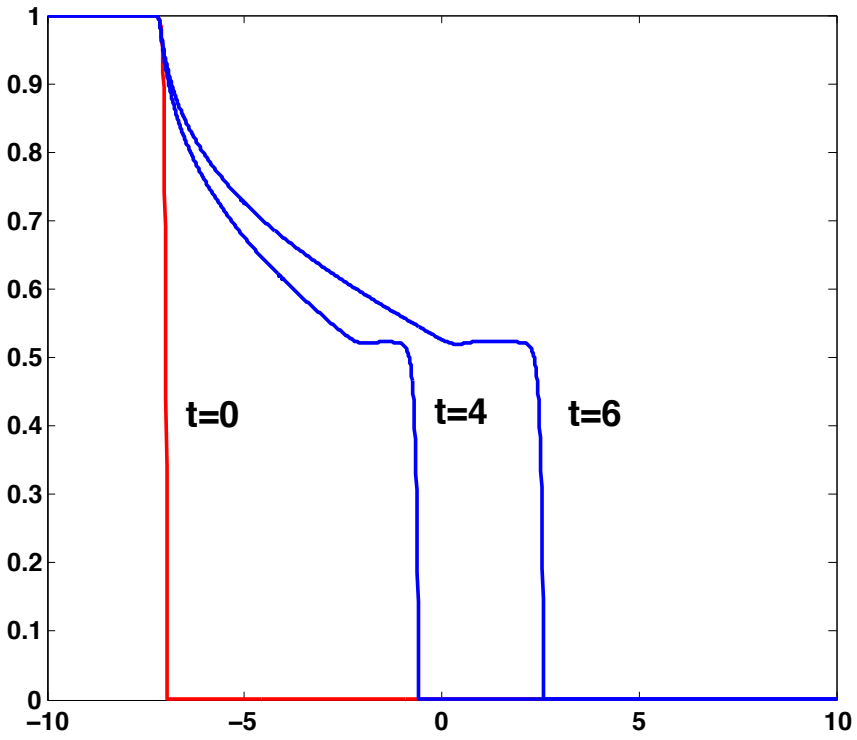
Idea works for more general constitutive laws

$$\psi(u) = -C_1 G(u) + C_2\sqrt{\kappa}\partial_x(\sqrt{\kappa}\partial_x u)); \quad G(u) \quad \text{bistable}$$

$$\frac{d}{du}\Big(\kappa(u)(\sec^2\theta - u)\Big) = \frac{K(\theta)}{2}G(u)$$

$$\kappa(u) = \frac{K(\theta)\int G(u)\,du}{4(\sec^2\theta - u)}, \quad 0 \le u \le 1$$

PDE simulations Rachel Levy



structure: rarefaction and leading (undercompressive) shock/TW from plateau $u = u_-$ to $u = 0$ at $x = st + x_0 < \infty$.

Traveling Waves

$$\partial_t u + \partial_x f(u) = \gamma \partial_x \left[H(u) G(u) \partial_x u \right] - \gamma C \partial_x \left[H(u) \partial_x m(u) \partial_x (m(u) \partial_x u) \right]$$

$$u = u(x - st), \;\; u(-\infty) = u_-, \;\; u(0) = 0, \;\; s = f(u_-)/u_-$$

$$-su + f(u) = \gamma H(u) G(u) u' - \gamma C H(u) (m(u)(m(u)u')')',$$

Note: constant of integration is zero
Write as first order system, $\beta = 1/(C\gamma)$ (multiply 3rd eqn by $m(u)$)

$$\begin{aligned} m(u)u' &= v \\ m(u)v' &= w \\ m(u)w' &= \tfrac{1}{C} G(u) v + \beta \frac{m(u)}{H(u)} (su - f(u)) \end{aligned}$$

Eliminate $m(u)$ to remove singularity at origin

ODE system - nondegenerate vector field

Eliminate $m(u)$: $m(u)\frac{d}{d\xi} = \frac{d}{d\eta}$, $u(\xi) = U(\eta), \ldots$

$$\begin{aligned} U' &= V \\ V' &= W \\ W' &= \tfrac{1}{C} G(U)V + \beta \frac{m(U)}{H(U)}(sU - f(U)) \end{aligned}$$

$(U, V, W) = (0, 0, 0)$ now a regular equilibrium

Seek solutions with $-\infty < \eta < \infty$
$(U, V, W)(-\infty) = (u_-, 0, 0)$, $(u, v, w)(\infty) = (0, 0, 0)$

Need real eigenvalues at origin: $\gamma > \gamma^*$: $Ca < Ca^*$

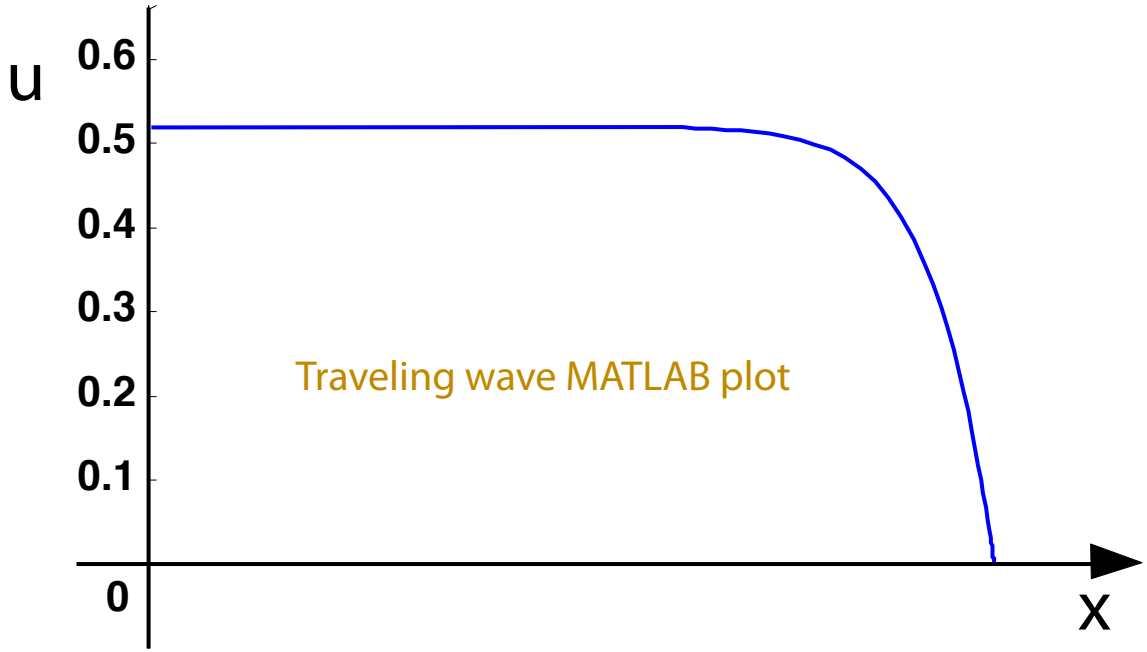
Shooting: 1-d unstable manifold from u_- to 2-d stable manifold at origin: $u_- = u_-(\beta)$.

Recover original variable $u(\xi) \to 0,\ \xi \to 0^-$

Transform back: $m(U(\eta))\, d\eta = d\xi$
$U(\eta) \sim ae^{\mu\eta}$ as $\eta \to \infty$, ($\mu < 0$: eigenvalue) implies

$$\xi = -\int_\eta^\infty U(y)\, dy = ae^{\mu\eta}/\mu$$

Thus, $u(\xi) = U(\eta) \sim \mu\xi$, as $\xi \to 0^-$, slope $\mu < 0$.



Summary

- Many applications with two-phase porous media flow
- Oil recovery context: oil/water interface; Lax shocks may be stable or unstable to 2-D perturbations; hyperbolic analysis gives condition for linear stability
- Yortsos and Hickernell (1989) traveling wave stability; most unstable wave number from dispersion relation tested by Zhengzheng Hu
- Phase field analysis for flow in capillary tube; undercompressive shocks, stationary compactons; degenerate diffusion traveling waves
- Hassanizadeh-Gray model
  degenerate diffusion-dispersion; sharp shocks