Stability Analysis and Solvers for Phase Transitions in Hydrate Formation

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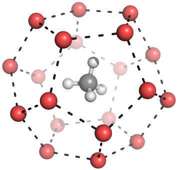
Motivation

Methane Hydrate:

- Ice-like crystal consists of methane gas trapped inside the water cage
- Exists under low temperature and high pressure
- Found in ocean sediments and polar regions
- Possible energy source in near future
- Environmental hazard



[D. Shin]

Siazik et al. [2017]

Deepwater Horizon [Jesslyn Shields]

Model

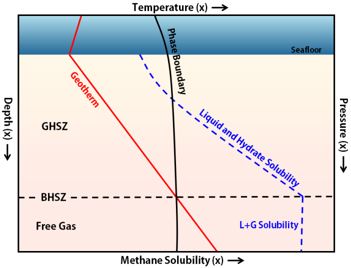
Two dynamic multiphase multicomponent flow models:

Liu-Fleming [2007]	Gupta-Helmig-Wohlmuth [2015]
basin scale	production time scale
allows saturated and unsaturated cases	does not allow unsaturated case
local thermodynamic equilibrium phase change	non-equilibrium phase change
porosity depends on stress	poro-elastic
salinity (NaCl)	free of any salinity
basis for simplified model allows well-posedness & numerical analysis[1]	-

[1] Gibson et al. [2014], Peszynska, Showalter, and Webster [2015], Peszynska, Hong, Torres, and Kim [2016]

Gas Hydrate Stability Zone (GHSZ)

- GHSZ; no gas is present
- Bottom of hydrate stability zone (BHSZ); $x = 0$
  - Depends on pressure, temperature, methane gas concentration, and activity of water[2]
  - Located at the three-phase equilibrium point
- Below of BHSZ; no hydrate formation



[2] Sloan [1998]

Maximum Solubility of Methane Gas

In the GHSZ, the maximum solubility of methane gas[3]

$$\chi^* \approx \chi^*(P, T, \text{salinity}, \text{rock type})$$

Assume:

- Pressure $\approx$ hydrostatic pressure,
- Temperature $\approx$ given by geothermal gradient,
- Salinity $=$ constant,
- Homogeneous rock type.

Then,

$$\chi^*(P(x,t), T(x), \text{salinity}, \text{rock type}) \approx \chi^*(x)$$

is a non-increasing function in x.

[3] Peszynska, Showalter, and Webster [2015]

Simplified Transport Model in Hydrate Zone[1]

$$\frac{\partial}{\partial t}\left(\phi(S_\ell \chi + S_h R_h\right) + \nabla \cdot \left(q\chi - \nabla \cdot (D_\ell^M \nabla \chi)\right) = \frac{f_M}{\rho_\ell}$$

Phase Equilibrium Condition:

$$\begin{cases} S_h = 0, & \text{if } \chi(x) \le \chi^*(x) \\ 0 \le S_h \le 1, & \text{if } \chi(x) > \chi^*(x) \\ S_h(\chi^*(x) - \chi(x)) = 0, & \text{for } x \in (0, D^{\max}) \end{cases}$$

- χ: Methane solubility (mass fraction in liquid phase)
- $S_{\ell,h}$: liquid/hydrate saturation; $S_\ell + S_h = 1$
- χ^*: Maximum solubility of methane; non-increasing function
- $R_h = \dfrac{\rho_h \chi_h^M}{\rho_\ell}$ (≈ 0.1203 kg/kg for realistic model)
- ϕ, D_ℓ^M: porosity and diffusion coefficient
- q: Darcy velocity in liquid

[1] Peszynska, Showalter, and Webster [2015]

Hydrate Zone: $S_\ell + S_h = 1$

Consider advective flow: $\boxed{u_t + q\chi_x = 0}$

where $u = (1 - S_h)\chi + S_h R_h$, the total methane content per mass of liquid phase.[1]

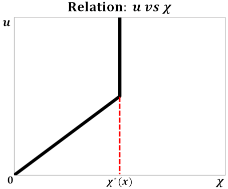
Challenge:

- $u(x;\chi)$ is a multivalued graph parametrized by x $(= -\text{depth})$

Approach:

- Consider the inverse of u:

$$\chi(x;u) = \begin{cases} u, & \text{if } u \le \chi^*(x) \\ \chi^*(x), & \text{if } u > \chi^*(x) \end{cases}$$



- $\chi(x;\cdot)$ is non-increasing in homogeneous sediment
- $\chi(\cdot;u)$ is increasing, concave, non-injective, but differentiable only a.e.

[1] Peszynska, Showalter, and Webster [2015], Gibson, Medina, Peszynska, and Showalter [2014]

Numerical Scheme

Solve numerically by the 1st order Godunov's scheme to get u.
Use local phase behavior solver to get χ and S from u.

- 1st order Godunov's scheme (Upwind):

(1) $$U_j^{n+1} = U_j^n - q\nu \left[F(\chi_j^n, \chi_{j+1}^n) - F(\chi_{j-1}^n, \chi_j^n) \right]$$

where $F(\chi_j^n, \chi_{j+1}^n) = \chi_j^n$ and $\nu = \dfrac{\tau}{h}$

- CFL condition: $|\nu \chi_u| \leq 1$
- Local phase behavior solver:

(2) $$\chi_j^n = \min\{U_j^n, \chi^*(x_j)\} \qquad (S_h)_j^n = \frac{U_j^n - \chi_j^n}{R_h - \chi_j^n}$$

- while $t^n \leq T$
    1. Given $U(x, t^n), \chi(x, t^n)$. $t^{n+1} = t^n + \tau$
    2. Compute $U(x, t^{n+1})$ using (1)
    3. Solve for $\chi(x, t^{n+1})$ and $S_h(x, t^{n+1})$ using (2)

Example 1

Consider the following problem:

$$\begin{cases} u_t + q\chi_x = 0, & x \in (0, D^{\max}),\ \ t > 0, \\ u(x,0) = u_L H(-x), & x \in (0, D^{\max}), \\ u(0,t) = u_L, \end{cases}$$

where

$$\chi(x;u) = \begin{cases} u, & \text{if } u \le \chi^*(x), \\ \chi^*(x), & \text{if } u > \chi^*(x). \end{cases}$$

[1] Peszynska, Hong, Torres, and Kim [2016]

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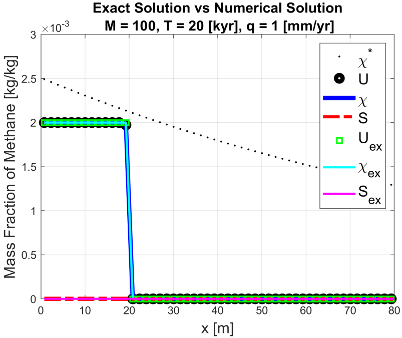
Ulleung Basin Site (UBGH2-11)[1] data:

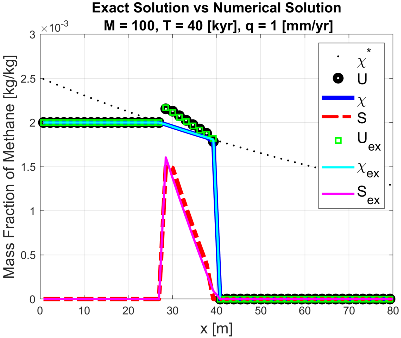
D_{ref}	P_{ref}	T_{ref}	Salinity	G_T	$D^{\max}$
2080 m	21.02 MPa	274.35 K	3.5%	0.12 K/m	154 m

[1] Peszynska, Hong, Torres, and Kim [2016]

Numerical Solution of Example 1

Comparison between the analytical solution[1] and the numerical solution





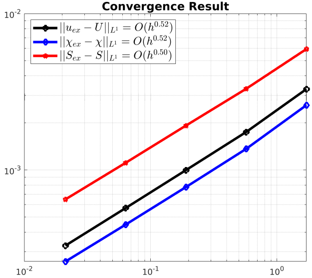
[1] Peszynska, Showalter, and Webster [2015]

Numerical Analysis of the Scheme

Rate of convergence:

- Well known for monotone finite different schemes for $u_t + \big(\chi(u)\big)_x = 0$:
  - $O(\sqrt{h})$ in L^1 for linear advection[4]
  - In L^1, convergence rate is no better than $O(\sqrt{h})$ even for a nonlinear flux[5]
  - In $W^{-1,1}$, convergence rate of $O(h)$ obtained[6]
  - $O(h)$ in $W^{-1,1}$ can be translated to $O(\sqrt{h})$ in L^1

Log-log plot



- Some result known for $u_t + \big(\chi(x;u)\big)_x = 0$ with monotone difference scheme:
  - In L^p_{loc}, convergence rate is $O(h)$ for Lax-Friedrichs scheme with smooth $\chi(\cdot, u)$ [7]
  - For $\chi(x;u) = k(x)f(u)$ with smooth f, convergence rate is $O(h)$ in L^1 for Godunov and EO fluxes[8]

[4] Lucier [1985], Tang and Teng [1995]

[5] Kruzhkov [1960], Kuznetsov [1976], Cockburn and Gremaud [1997], Sabac [1997]

[6] Tadmor [1991], Nessyahu and Tadmor [1992], Nessyahu, Tadmor, and Tassa [1994]

[7] Karlsen [2003], Karlsen and Towers [2004]

[8] Towers [2000]

Stability analysis

Theorem [Peszynska, Shin, 2019][9]

Assume $\chi \in C^2((0, D^{\max}) \times \mathbb{R}_+ \cup \{0\})$. Numerical scheme is weakly total-variation stable. In particular,

(A) $$TV(U^n) \leq C_1(T)TV(U^0) + C_2(T).$$

Further,

(B) $$TV_T(U^n) \leq C(T)$$

where $C(T)$ is some constant depends on T and $TV(U^0)$.

[9] Peszynska, Shin [2019], *manuscript in preparation*

Stability analysis

Theorem [Peszynska, Shin, 2019][9]

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Further,

(B) $$TV_T(U^n) \leq C(T)$$

where $C(T)$ is some constant depends on T and $TV(U^0)$.

Challenges in proof

- Numerical scheme is not TVD
- $\chi(x; u)$ is not separable
- Work with source term $u_t + \chi_u(x; u)u_x = -\chi_x(x; u)$ for smooth χ

[9] Peszynska, Shin [2019], *manuscript in preparation*

Proof outline of (A)

$$\boxed{U_j^{n+1} = U_j^n - \nu\left[\chi_j^n - \chi_{j-1}^n\right]}$$

Assume $\chi \in C^2((0, D^{\max}) \times \mathbb{R}_+ \cup \{0\})$. Let $\Delta U_j^n = U_j^n - U_{j-1}^n$. Subtract the scheme at $j-1$ from j to get

$$\Delta U_j^{n+1} = \Delta U_j^n - \nu\left[\chi_j^n - \chi_{j-1}^n\right] + \nu\left[\chi_{j-1}^n - \chi_{j-2}^n\right].$$

Substitute $\chi_i^n - \chi_{i-1}^n$ for $i = j, j-1$ with

$$\chi_i^n - \chi_{i-1}^n \approx \chi_u(x_i, \overline{U}_i^n)(U_i^n - U_{i-1}^n) + \chi_x(\overline{x}_i, U_{i-1}^n)h$$

using the mean value theorem. Then rearrange to get

$$\begin{aligned}\Delta U_j^{n+1} = \Delta U_j^n\left(1 - \nu\chi_u(x_j, \overline{U}_j^n)\right) &- \nu\chi_u(x_{j-1}, \overline{U}_{j-1}^n)\Delta U_{j-1}^n \\ &- \tau\Big[\underbrace{\chi_x(\overline{x}_j, U_{j-1}^n) - \chi_x(\overline{x}_{j-1}, U_{j-2}^n)}_{A_1}\Big].\end{aligned}$$

Use the mean value theorem to rewrite A_1.

Proof outline of (A)

Take the absolute value and apply the triangle inequality. Then take the sum over $j \in \mathbb{Z}$. With CFL condition $|\nu\chi_u| \leq 1$,

$$TV(U^{n+1}) \leq TV(U^n) - \sum_{j\in\mathbb{Z}} \nu\chi_u(x_j, \overline{U}_j^n)\left|\Delta U_j^n\right| + \sum_{j\in\mathbb{Z}} \nu\chi_u(x_{j-1}, \overline{U}_{j-1}^n)\left|\Delta U_{j-1}^n\right|$$

$$+ \tau\|\chi_{xu}\|_\infty \sum_{j\in\mathbb{Z}}\left|\Delta U_{j-1}^n\right| + 2\tau\|\chi_{xx}\|_\infty \sum_{j\in\mathbb{Z}} h$$

Re-indexing results

$$TV(U^{n+1}) \leq TV(U^n)(1+\alpha\tau) + \beta\tau \qquad \text{where } \alpha, \beta > 0$$

We can obtain the TV bound:

$$TV(U^n) \leq TV(U^0)(1+\alpha\tau)^n + \beta\tau\sum_{k=0}^{n-1}(1+\alpha\tau)^k$$

Evaluate the finite series: $\displaystyle\sum_{k=0}^{n-1}(1+\alpha\tau)^k = \frac{(1+\alpha\tau)^n - 1}{\alpha\tau}$

Bernoulli's inequality: $(1+\alpha\tau)^n \leq e^{n\alpha\tau} = e^{\alpha T}$ where $n\tau = T$

Proof outline of (B)

$$TV_T(U^n) = \sum_{n=0}^{T/\tau} \left[\tau TV(U^n) + \|U^{n+1} - U^n\|_1 \right]$$

To obtain a bound for $\|U^{n+1} - U^n\|_1$, we rewrite the scheme as

$$U_j^{n+1} - U_j^n = -\nu \left[\chi_j^n - \chi_{j-1}^n \right]$$

Following a similar pattern as in the proof of (A), we get

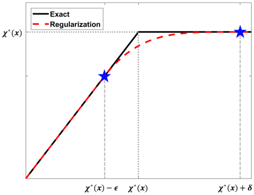
$$\sum_{j\in\mathbb{Z}} \left| U_j^{n+1} - U_j^n \right| h \leq \tau(\|\chi_u\|_\infty TV(U^n) + D^{\max}\|\chi_x\|_\infty)$$

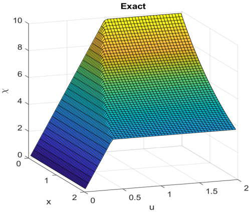
Then using (A), we can prove (B).

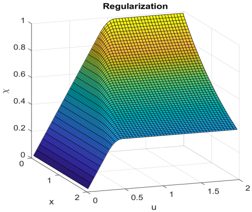
Understanding the "blow-up" behavior

Behavior of $\chi(x; u)$ in our problem. (Note: Theorem requires $\chi \in C^2$)

- Main challenge: $\chi(\cdot; u)$ is only piecewise smooth
- Regularize $\chi \approx \chi^{\epsilon,\delta,n}$







Note: $\|\chi - \chi^{\epsilon,\delta,5}\|_\infty = O(\epsilon)$ and $\|\chi - \chi^{\epsilon,\delta,5}\|_{L_1} = O(\epsilon^2)$ with $\delta, h = O(\epsilon)$ from computational experiments

- Quasilinear form:

$$u_t^{\epsilon,\delta,n} + \chi_u^{\epsilon,\delta,n}(x; u^{\epsilon,\delta,n})u_x^{\epsilon,\delta,n} = -\chi_x^{\epsilon,\delta,n}(x; u^{\epsilon,\delta})$$

- $-\chi_x^{\epsilon,\delta,n}(x;\cdot) > 0$ leads to the blow-up in spite of $\chi^{\epsilon,\delta,n}(\cdot, u^{\epsilon,\delta,n})$ concave

One other way to understand convergence

Convergence using the regularized flux

$$\|u - U\|_{L_1} \leq \|u - u^{\epsilon,\delta,n}\|_{L_1} + \|u^{\epsilon,\delta,n} - U^{\epsilon,\delta,n}\|_{L_1} + \|U^{\epsilon,\delta,n} - U\|_{L_1}.$$

If we have

$$\|\chi_x - \chi_x^{\epsilon,\delta,n}\|_\infty + \|\chi_u - \chi_u^{\epsilon,\delta,n}\|_\infty + \|u_x^{\epsilon,\delta,n}\|_\infty \to 0 \text{ as } \epsilon, \delta \to 0^+$$

then

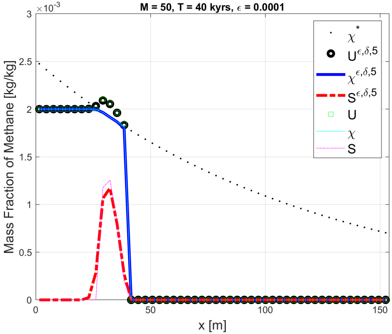
$$\|u - u^{\epsilon,\delta,n}\|_{L_1} \to 0 \text{ as } \epsilon, \delta \to 0^+.$$

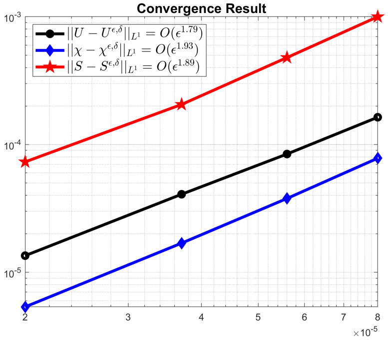
Numerical experiments show:

- $\|u^{\epsilon,\delta,n} - U^{\epsilon,\delta,n}\|_{L_1} = O(h)$
- $\|U^{\epsilon,\delta,n} - U\|_{L^1} = O(\epsilon^{1.79})$

Example 2: Advection with regularized flux $u_t^{\epsilon,\delta,5} + q\chi_x^{\epsilon,\delta,5} = 0$

Comparison between numerical solutions with exact and regularized fluxes:

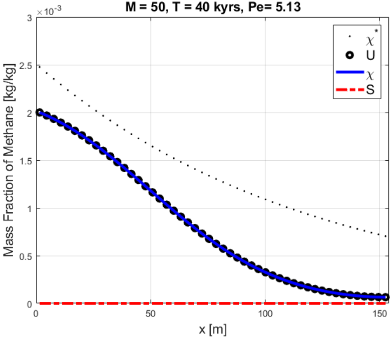


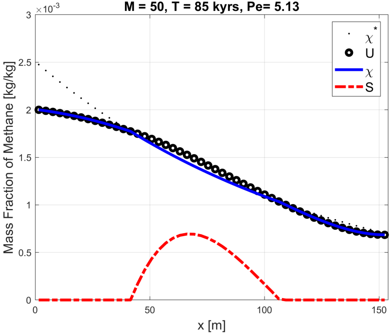


$\|u_{\text{fine}}^{\epsilon,\delta,5} - U^{\epsilon,\delta,5}\|_{L^1}$	$\|\chi_{\text{fine}}^{\epsilon,\delta,5} - \chi^{\epsilon,\delta,5}\|_{L^1}$	$\|S_{\text{fine}}^{\epsilon,\delta,5} - S^{\epsilon,\delta,5}\|_{L^1}$
$O(h)$	$O(h)$	$O(h)$

$\star$ Note that the regularized flux converges to the exact flux at the rate of ϵ^2 in L_1-norm.

Example 3: Advection-diffusion $u_t + q\chi_x - D_\ell^M \chi_{xx} = 0$



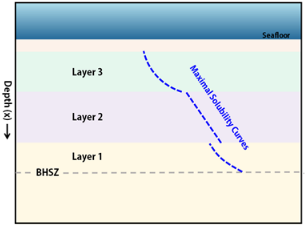


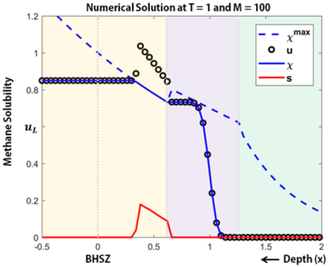
Convergence (as expected, 1st order scheme, smooth solution)

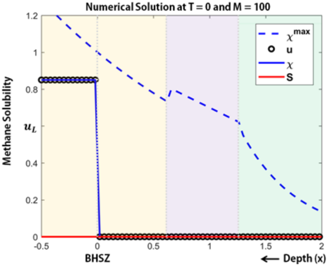
$\|U_{\text{fine}} - U_{AD}\|_{L_1}$	$\|\chi_{\text{fine}} - \chi_{AD}\|_{L_1}$	$\|S_{\text{fine}} - S_{AD}\|_{L_1}$
$O(h^{1.1})$	$O(h^{1.04})$	$O(h^{1.07})$

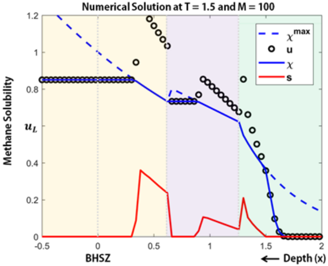
Example 4: Heterogeneous Rock Types

Advection flow (model problem motivated by Daigle and Dugan [2011])







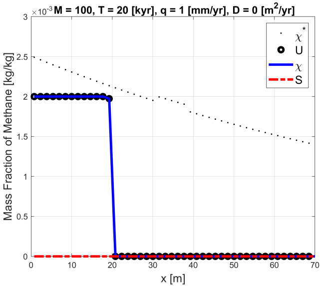


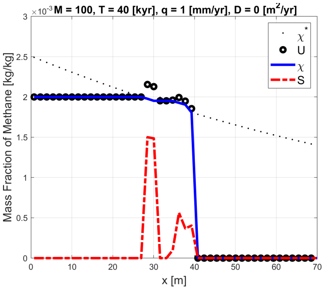
Example 4: Heterogeneous Rock Types

Layer profile

x [m]	$[0, 30]$	$(30, 40)$	$[40, 154]$
Layer Type	UBGH2-11	UBGH2-2_1	UBGH2-11

Numerical solution to advection flow:





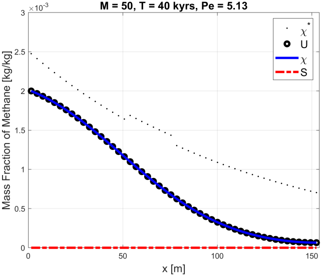
$\|\|U_{\text{fine}} - U\|\|_{L^1}$	$\|\|\chi_{\text{fine}} - \chi\|\|_{L^1}$	$\|\|S_{\text{fine}} - S\|\|_{L^1}$
$O(h^{0.55})$	$O(h^{0.57})$	$O(h^{0.52})$

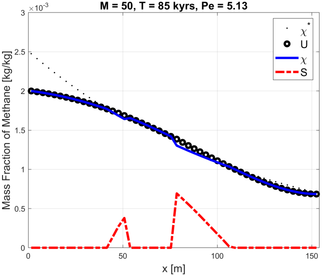
Example 4: Heterogeneous Rock Type

Layer profile

x [m]	$[0, 60]$	$(60, 80)$	$[80, 154]$
Layer Type	UBGH2-11	UBGH2-2_1	UBGH2-11

Numerical solution to advection-diffusion flow





$\lVert U_{\text{fine}} - U_{AD} \rVert_{L^1}$	$\lVert \chi_{\text{fine}} - \chi_{AD} \rVert_{L^1}$	$\lVert S_{\text{fine}} - S_{AD} \rVert_{L^1}$
$O(h^{1.07})$	$O(h^{1.12})$	$O(h^{1.23})$

Future work

- Work with more realistic model that account for viscous and capillary effects, pressure compresibility, relative permeability and capillary pressure
- Extend phase package from Peszynska et al. [2016] to gas zone
- Contribute to the github package for MH
- Implement in higher dimensions

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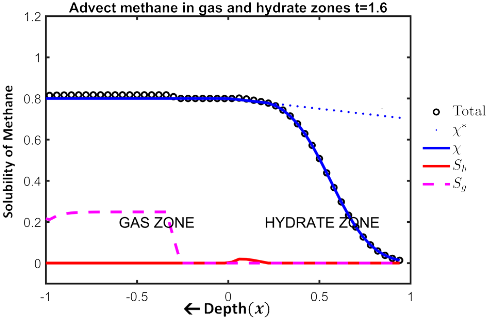
Gas and Hydrate Zone $S_\ell + S_h + S_g = 1$

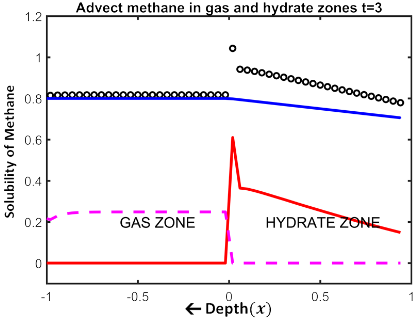
Inspired by Liu and Flemings [2007]:

$$u_t + \nabla \cdot (q\chi + q_g R_g) = 0 \qquad \text{with } u = S_\ell \chi + S_h R_h + S_g R_g$$

- Assumptions:
  - Free gas can move if $S_g > S_{g,res}$
  - $q >> q_g > 0$
  - Neglect relative permeability, capillary pressure, and pressure compressibility for this example
- Challenges:
  - No analytical solution exists
  - Account viscous and capillary effects and pressure compressibility
  - Unknown physical behavior of methane gas and hydrate in gas and hydrate zone
- Use Godunov's scheme and local phase behavior solver which accounts both S_h and S_g
- Compare the result with fine grid solution

Numerical Solution





Convergence

$\|U_{\text{fine}} - U\|_{L^1}$	$\|\chi_{\text{fine}} - \chi\|_{L^1}$	$\|S_{h,\text{fine}} - S_h\|_{L^1}$	$\|S_{g,\text{fine}} - S_g\|_{L^1}$
$O(h^{0.59})$	$O(h^{0.56})$	$O(h^{1.21})$	$O(h^{0.62})$