Numerical Approximation for a Model of Methane Hydrates

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PNWNAS, Seattle.

October 19, 2013

[N. Gibson, P. Medina, M. Peszynska, R. Showalter, *Evolution of phase transition in methane hydrate*, JMAA, V. 409, Issue 2 (2014), 816-833.]

Partially supported by NSF DMS-1115827 "Hybrid Modeling in porous media"

Acknowledgements

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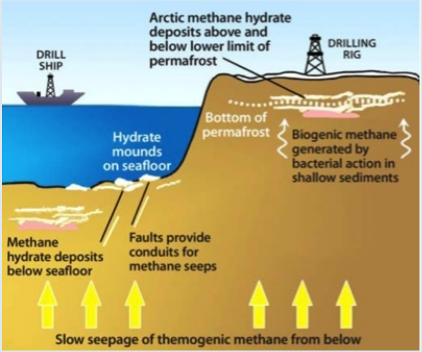
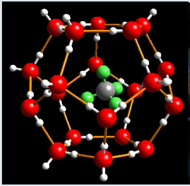
Partially supported by NSF DMS-1115827 “Hybrid Modeling in porous media”, PI: Malgorzata Peszynska

Motivation





[Images from DOE-NETL]

$P(x)$ pressure (known)
$T(x)$ temperature (known)

Phases:

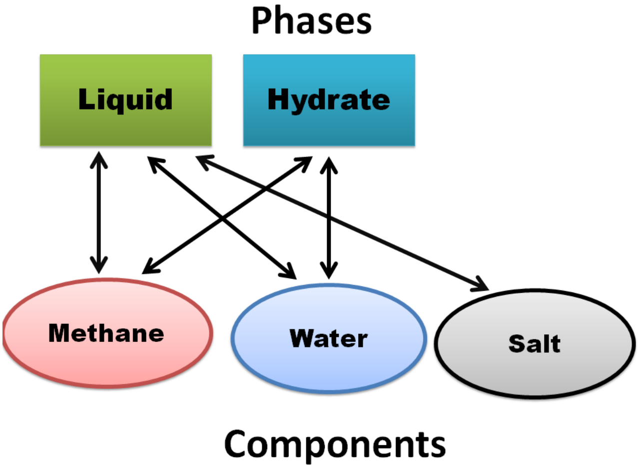
- Liquid
- Hydrate
  - stable if P high, T low

Components

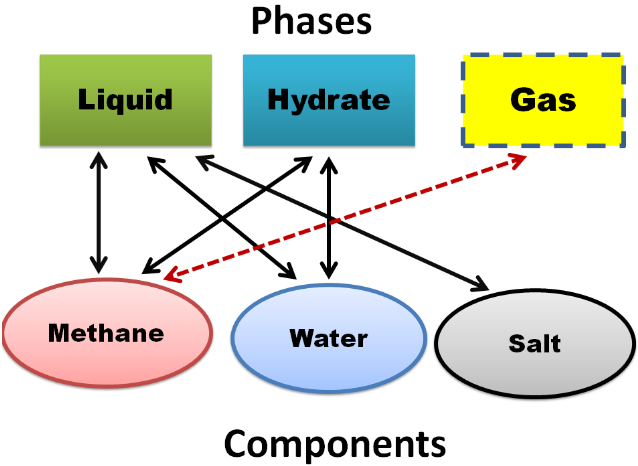
- CH_4
- H_2O

[References at the end of the talk]

Phases and components



Phases and components (no gas phase in this talk)



Phases

Liquid

Hydrate

Gas

Methane

Water

Salt

Components

Conservation of mass for CH_4 component

$$\frac{\partial}{\partial t}(\phi_0 S_l \rho_l v_{lM} + \phi_0 S_h \rho_h v_{hM}) - \nabla \cdot (D_{lM} \rho_l \nabla v_{lM}) = f_M$$

ϕ_0 : porosity

D_{lM} : diffusivity

S_l, S_h : saturations, $S_l = 1 - S_h$

ρ_l, ρ_h : densities

v_{lM} : fraction of CH_4 in liquid

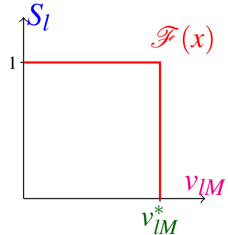
v_{hM} : fraction of CH_4 in hydrate (known)

f_M : external source of CH_4

Assumption: v_{lS} is known

Unknowns: S_l, v_{lM}

Need $(S_l, v_{lM}) \in \mathscr{F}(x)$



Conservation of mass for CH_4 component

$$\frac{\partial}{\partial t}(\cancelto{1}{\phi_0} S_l \rho_l v_{lM} + \cancelto{1}{\phi_0}\, S_h\, \rho_h v_{hM}) - \nabla \cdot (\cancelto{1}{D_{lM}} \rho_l \nabla v_{lM}) = f_M$$

ϕ_0 : porosity=1

D_{lM} : diffusivity (constant)=1

S_l, S_h : saturations, $S_l = 1 - S_h$

ρ_l, ρ_h : densities (assumed constant)

v_{lM} : fraction of CH_4 in liquid

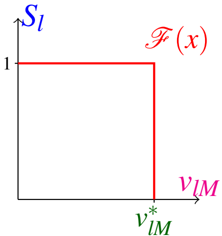
v_{hM} : fraction of CH_4 in hydrate (known)

f_M : external source of CH_4

Assumption: v_{lS} is known

Unknowns: S_l, v_{lM}

Need $(S_l, v_{lM}) \in \mathscr{F}(x)$

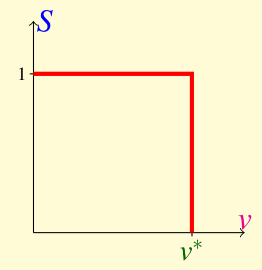


Solubility constraint

$$\frac{\partial}{\partial t}(Sv + R(1-S)) - \nabla \cdot (\nabla v) = f$$

Solubility constraint

$$\begin{cases} v \leq v^*, & S = 1, \\ v = v^*, & S \leq 1, \\ (v^* - v)(1 - S) = 0. \end{cases}$$

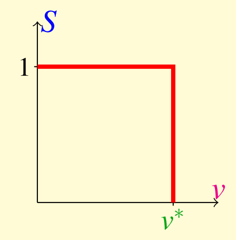


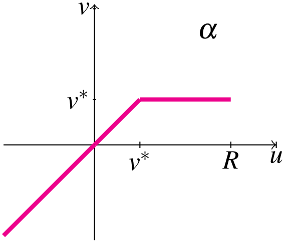
...this is a

Nonlinear Complementarity Constraint (NCC)

Towards an abstract evolution equation...

$$\frac{\partial}{\partial t}\underbrace{(Sv+R(1-S))}_{u}-\Delta v=f$$





Rewrite as $\begin{cases} \dfrac{\partial u}{\partial t}-\Delta v=f \\ v\in\alpha(u) \end{cases}$

Abstract evolution equation

$$\begin{aligned} \frac{\partial u}{\partial t} - \Delta v =& f, \quad v \in \alpha(u) \text{ on } \Omega \times (0,T) \\ v =& 0, \text{ on } \partial\Omega \times (0,T) \\ u(\cdot,0) =& u_0(\cdot), \text{ on } \Omega. \end{aligned}$$

- Abstract IVP with $\frac{du}{dt} + Au = f$ with $A = -\triangle \circ \alpha$
  - A is *maximal monotone*
  - A is a sub-gradient

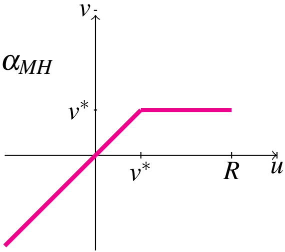
Two notions of solution:

- $u \in C([0,T], L^1(\Omega))$ with $v(t) \in W_0^{1,1}(\Omega)$, $\triangle v(t) \in L^1(\Omega)$,
- $u \in W^{1,1}([0,T], \mathscr{V}')$, $v(t) \in \mathscr{V}$, with $\mathscr{V} = H_0^1(\Omega)$.

Need measurable family of graphs, $\alpha = \alpha(x)$

- Measurable family of convex functions
- Normal convex integrand
- Comparison principle

Examples: $\alpha = \alpha_{MH}, \alpha_{ST}, \alpha_{PM}$

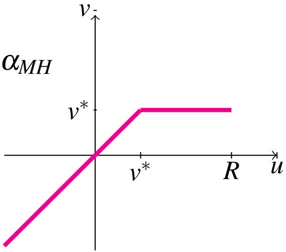


Methane hydrate:

$$\alpha_{MH}(x;u) = (u - v^*(x))_- + v^*(x),\ u \leq R$$

Looks like α_{ST}

Examples: $\alpha = \alpha_{MH}, \alpha_{ST}, \alpha_{PM}$



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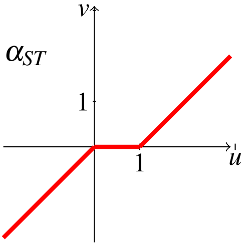


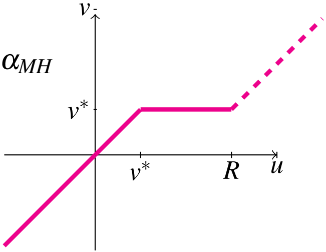
Stefan free-boundary problem:

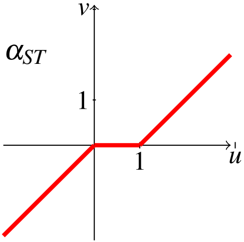
$\alpha_{ST}(u) = u_- + (u-1)_+$

(Much is known,

$\alpha_{ST} \neq \alpha_{ST}(x)$)

Examples: $\alpha = \alpha_{MH}, \alpha_{ST}, \alpha_{PM}$





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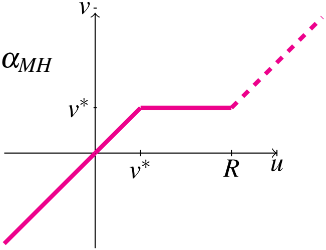

Methane hydrate:

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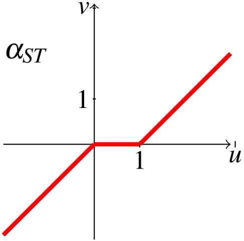


Stefan free-boundary problem:

$\alpha_{ST}(u) = u_- + (u-1)_+$

(Much is known,

$\alpha_{ST} \neq \alpha_{ST}(x)$)

Porous medium equation (PME)

Much is known also for PME: $\alpha = \alpha_{PM}(u) = |u|u^{m-1}$

- $m > 1$ slow diffusion
- $0 < m < 1$ fast diffusion

Related work (on Stefan problem)

Stefan problem= “ice-water phase transition”

Elliot’81,. . . , Jerome-Rose’82,. . . , Nochetto-Verdi’88, . . . , Rulla-Walkington’96, Rulla’96.

FE formulation for $\alpha = \alpha_{MH}(x, \cdot)$

FE formulation

Consider a triangulation $\mathscr{T}_h$ for Ω.
$\mathscr{V}_h \subset \mathscr{V}$ be the linear finite element space on $\mathscr{T}_h$

Scheme: Find $v_h^n \in \mathscr{V}_h$ at t_n $(n > 0)$

$$\begin{cases} (u_h^n, \psi) + \tau(\nabla v_h^n, \nabla \psi) = (u_h^{n-1}, \psi), \forall \psi \in \mathscr{V}_h \\ u_h^n \in \alpha_h^{-1}(v_h^n) \\ (u_h^0, \psi) := (u_0, \psi) \end{cases}$$

Algebraic system

$$v_h^n \equiv \mathbf{v}^n \in \mathbb{R}^M$$

$(w, \Phi) \longrightarrow (w, \Phi)_h$
(mass lumping)

Discussion

- Convergence results in $L^2(Q)$ [Nochetto-Verdi, 1988]
- Selection of $\alpha^{-1}(v_h(x_j))$ is not unique.
  Duality argument helps.

Discrete problem, use $A_h = M^{-1}K$

$$\begin{cases} \mathbf{u}^n + \tau \mathbf{A}_h \mathbf{v}^n = \mathbf{u}^{n-1} \\ \langle v_j^n, u_j^n \rangle \in \alpha^{-1}(x_j; \cdot) \end{cases}$$

Solver: Semismooth Newton method for NCC

Uniqueness of numerical solution

Lemma [GMPS'13]

For every $n > 0$ there is a unique solution $\mathbf{v}^n \in \mathbb{R}^M$ of the discrete problem for $\alpha^{-1} = \alpha_{MH}^{-1}(x;\cdot)$. It is the unique minimizer of the appropriate functional $\Psi(\mathbf{v})$ for which the discrete problem is the Euler-Lagrange condition.

Let $\Phi(\mathbf{v}) := \sum_j \phi_j(v_j)$, where $\phi_j(\lambda) = \frac{1}{2}\lambda^2 + I_{(-\infty, v^*(x_j)]}(\lambda)$.
Take $\Psi(\mathbf{v}) = \frac{1}{2}\tau \mathbf{v}\mathbf{A_h}\mathbf{v}^{\mathbf{T}} + \Phi(\mathbf{v})$ and consider $\partial\Psi(\mathbf{v})$.

Corollary

The discrete scheme is uniquely solvable for α_{ST}^{-1}

Comparison principle

Lemma [GMPS'13]

Let $\mathbf{u}^{(1)}, \mathbf{u}^{(2)}$ with the corresponding $\mathbf{v}^{(1)}, \mathbf{v}^{(2)}$ satisfy

$$\mathbf{u} + \tau \mathbf{A}_h \mathbf{v} = \mathbf{f}, \quad u_j \in \alpha_j^{-1}(v_j) \quad (j = 1, 2, \dots, M)$$

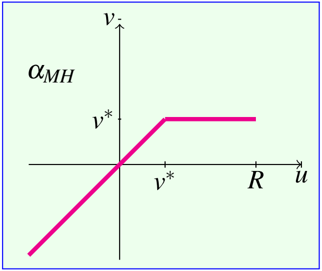
for $\mathbf{f} = \mathbf{f}^{(1)}, \mathbf{f}^{(2)}$. Let also $v_j^{(1)} - v_j^{(2)} = 0$ for boundary indices j. Then

$$\sum_{j=1}^{M} (\mathbf{u}^{(1)} - \mathbf{u}^{(2)})_+ \le \sum_{j=1}^{M} (\mathbf{f}^{(1)} - \mathbf{f}^{(2)})_+$$

Comments:

- We don't require α or α^{-1} to be single-valued
- **Multivalued case**: use Yosida approximation of α and α^{-1}

Semismooth Newton for $u \in \alpha^{-1}(v)$ as an NCC



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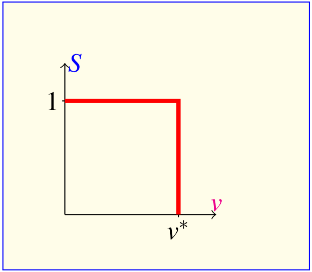


$$\langle u, v\rangle \in \alpha_{MH} \equiv \min(v^*(x) - v, 1 - S) = 0$$

Time step

$$\mathbf{u}^n + \tau \mathbf{A}_h \mathbf{v}^n = \mathbf{u}^{n-1}$$
$$\langle u_j^n, v_j^n\rangle \in \alpha(x_j;\cdot),\ \forall j$$

$\Leftrightarrow$

Stationary problem

$$\begin{cases} \mathbf{u} + \tau \mathbf{A}_h \mathbf{v} = \mathbf{b} \\ \min(v_j^*(x) - v_j, 1 - S_j) = 0,\ \forall j \end{cases}$$

Semismooth Newton converges *superlinearly* for the MH problem

[Ulbrich, 2011], [Ben Gharbia, Gilbert and Jaffre, 2011]

Convergence of the scheme in u, v and S

$1/h$	$1/\tau$	N_{it}	$e_{u,2}$	$r_{u,2}$	$e_{u,1}$	$r_{u,1}$	$e_{v,2}$	$r_{v,2}$	$e_{v,1}$	$r_{v,1}$	e_q	r_q
256	2560	2	3.45e-03	0.561	1.56e-04	1.028	6.77e-04	0.763	6.40e-05	1.014	7.07e-04	0.785
512	5120	2	2.27e-03	0.605	7.39e-05	1.084	3.86e-04	0.811	3.03e-05	1.080	3.98e-04	0.827
128	12800	2	4.50e-03	0.554	1.88e-04	1.043	2.19e-04	0.990	1.86e-05	1.228	5.33e-04	0.967
256	25600	2	2.96e-03	0.604	8.88e-05	1.087	1.19e-04	0.875	8.26e-06	1.172	2.68e-04	0.995
32	1024	2	9.18e-03	0.636	8.21e-04	1.182	1.18e-03	1.330	1.65e-04	1.684	1.98e-03	1.013
64	4096	2	5.98e-03	0.619	3.67e-04	1.160	4.86e-04	1.280	5.24e-05	1.655	9.88e-04	1.000

$$\tau = \frac{h}{10}, \frac{h}{100}, h^2$$

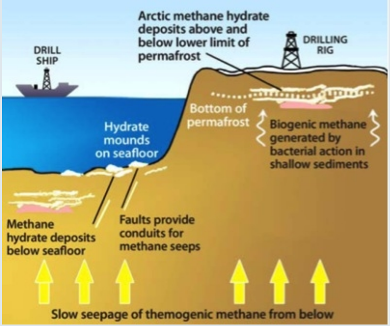
$$e_{u,2} \approx O(h^{1/2})$$

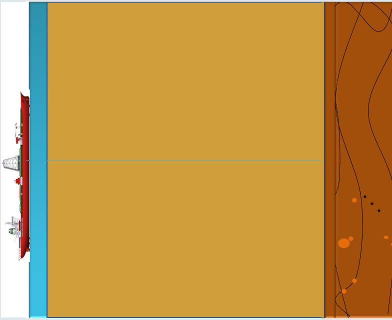
$$e_{u,1} \approx O(h), \quad e_{v,2} \approx O(h), \quad e_{v,1} \approx O(h) \text{ and } e_q \approx O(h)$$

	constant				affine				non-affine			
$1/h$	$e_{S,2}$	$r_{S,2}$	$e_{S,1}$	$r_{S,1}$	$e_{S,2}$	$r_{S,2}$	$e_{S,1}$	$r_{S,1}$	$e_{S,2}$	$r_{S,2}$	$e_{S,1}$	$r_{S,1}$
64	2.91e-03	0.537	1.32e-04	1.001	7.89e-03	0.519	5.24e-04	0.994	5.27e-03	0.525	2.91e-04	1.001
128	1.97e-03	0.559	6.43e-05	1.039	5.41e-03	0.546	2.56e-04	1.032	3.58e-03	0.556	1.41e-04	1.041
256	1.30e-03	0.602	3.03e-05	1.084	3.56e-03	0.600	1.21e-04	1.084	2.36e-03	0.603	6.66e-05	1.086

$$e_{S,2} \approx O(h^{1/2}), \quad e_{S,1} \approx O(h)$$

Simulations





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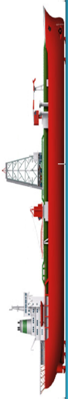
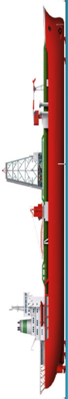


Sim 1: Undersaturated case with Methanogenesis

Sim 2: Saturated case, with hydrate melting

Sim 1:Undersaturated case with Methanogenesis



$$\Omega = (0,1)$$

$$T = 0.2$$

$$M = 64$$

$$\Delta t = 10(\Delta x)^2$$

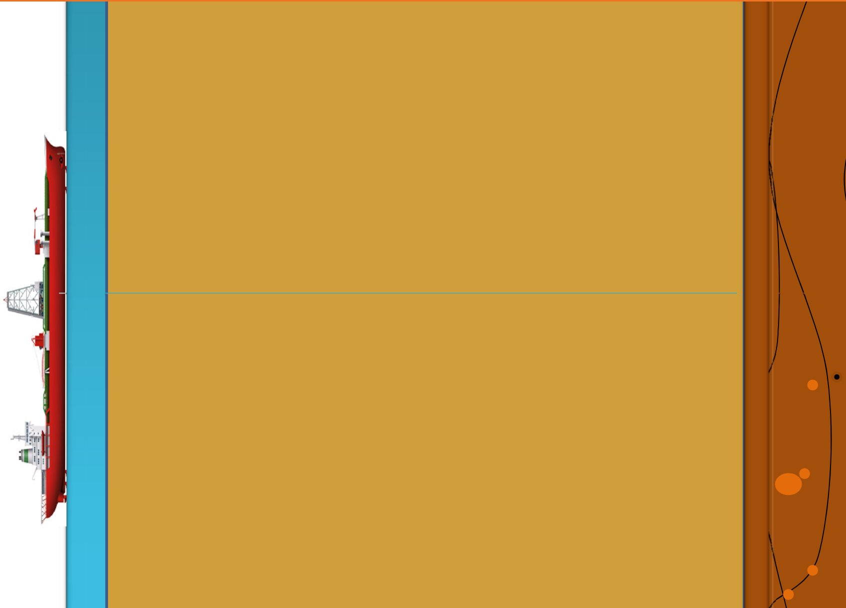
$$v^* = 0.5(x^2+1)$$

$$u(x,0) \quad \text{linear}$$

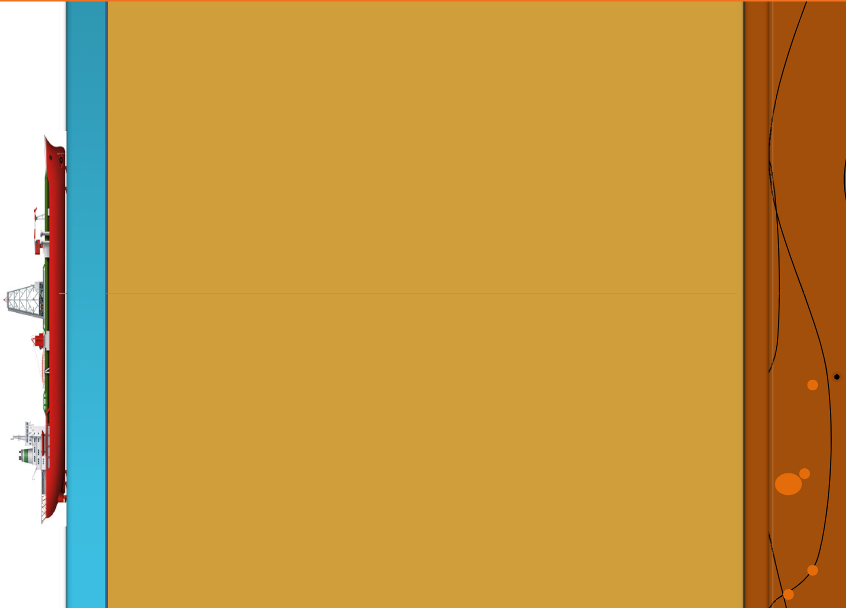
$$v(0,t) = 0.7v^*(0),$$
$$v(1,t) = 0.7v^*(1), \quad t > 0$$

Methanogenesis $\approx$ point source

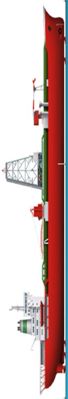
Sim 1: Undersaturated case with Methanogenesis. Initial Condition, $t = 0$



Sim 1: Undersaturated case with Methanogenesis. $t > 0$



Sim 2: Saturated case, with hydrate melting



$$\Omega = (0,1)$$

$$T = 0.1$$

$$M = 50$$

$$\Delta t = 10(\Delta x)^2$$

$$v^*(x) = 0.25(x+1)$$

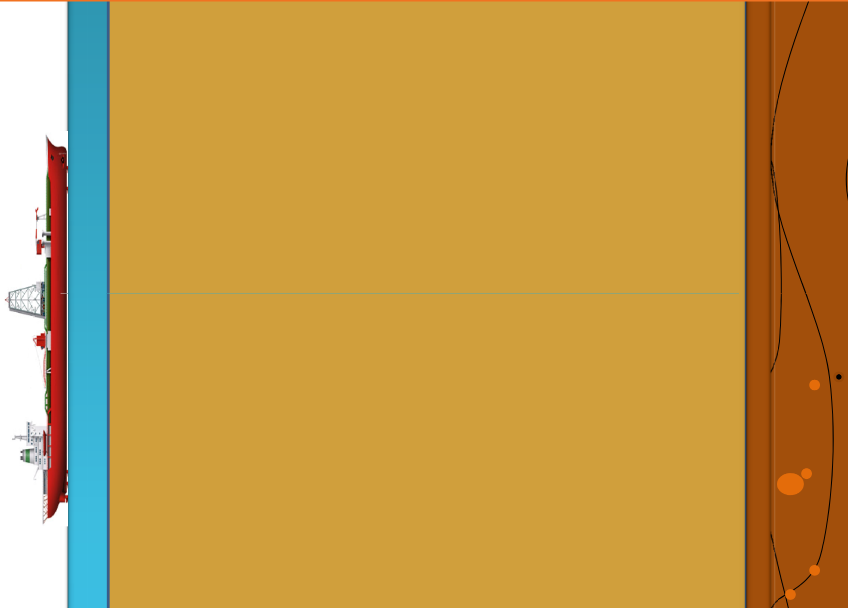
$$u(x,0) = \text{ equilibrium, slight perturbation}$$

$$v(0,t) = 0,$$
$$v(1,t) = v^*(1), \quad t > 0$$

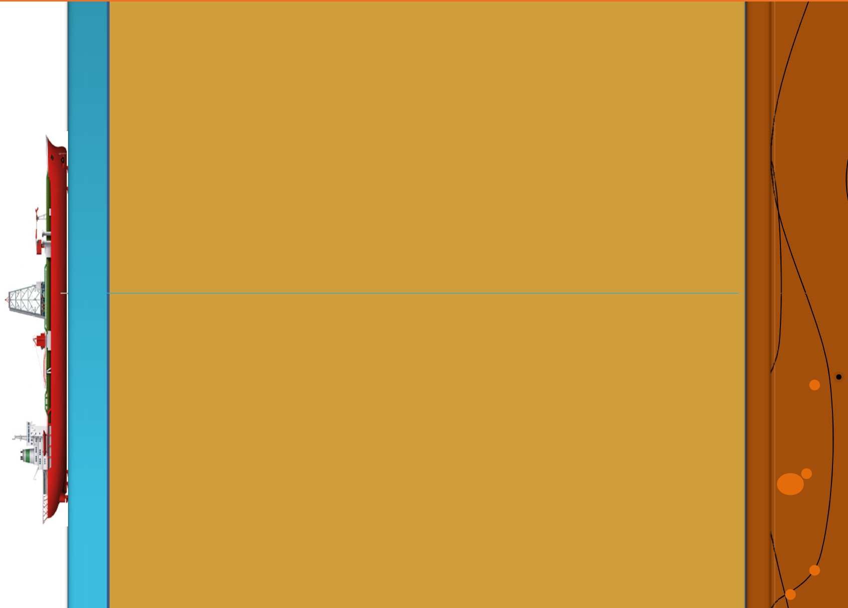
$$f = 0$$

Sim 2: Saturated case, with hydrate melting.

Initial condition, $t = 0$



Simu 2: Saturated case, with hydrate melting.
$t > 0$



Summary and future work

- MH problem $\approx$ Stefan problem.
- MH problem $\supsetneqq$ Stefan problem with $\alpha = \alpha(x, \cdot)$
- Convergence for MH $\approx$ convergence for Stefan
- Semismooth Newton solver works as it should.
  - No regularization needed!!!
- NCC form $\equiv$ “variable switching” (industry standard for multicomponent-flow)
- Can solve Stefan problem with semismooth Newton method $u \in \alpha_{ST}^{-1}(v) \equiv u - v - \max(0, \min(u, 1)) = 0$

Future work

- Implementation in 2D/3D
- Evolution in the gas zone.
- Include salinity as a variable (extra equation needed)
- More model extensions (variables P and T), even more equations needed.

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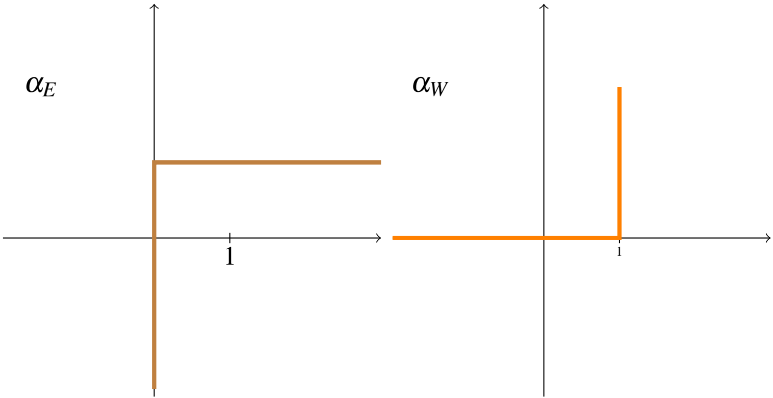
Additional examples (“Elbow” and “Woble” graphs)

Neither α or α^{-1} is a function!!



Convergence in u and v (Elbow)

			error	rate	error	rate	error	rate	error	rate	error	rate
$1/h$	$1/\tau$	N_{it}	$e_{u,2}$	$r_{u,2}$	$e_{u,1}$	$r_{u,1}$	$e_{v,2}$	$r_{v,2}$	$e_{v,1}$	$r_{v,1}$	e_q	r_q
256	2560	2	1.03e-02	0.540	3.61e-04	1.038	1.19e-03	0.785	1.16e-04	1.057	6.40e-04	1.073
512	5120	2	6.81e-03	0.601	1.70e-04	1.089	6.73e-04	0.828	5.72e-05	1.026	3.00e-04	1.094
128	12800	2	1.47e-02	0.546	7.28e-04	1.037	1.23e-03	0.966	2.35e-04	1.001	1.48e-03	1.016
256	25600	2	9.69e-03	0.602	3.42e-04	1.089	6.29e-04	0.961	1.17e-04	1.002	7.19e-04	1.040
32	1024	2	2.90e-02	0.516	2.80e-03	0.953	5.25e-03	0.945	9.94e-04	0.936	5.42e-03	0.800
64	4096	2	1.93e-02	0.591	1.35e-03	1.058	2.62e-03	1.003	4.88e-04	1.026	2.78e-03	0.964

$$\tau = \frac{h}{10}, \frac{h}{100}, h^2$$

$$e_{u,2} \approx O(h^{1/2})$$

$$e_{u,1} \approx O(h), \quad e_{v,2} \approx O(h), \quad e_{v,1} \approx O(h) \text{ and } e_q \approx O(h)$$

Thanks!