Numerical Modeling of Methane Hydrate Evolution

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Joint work with F. P. Medina, M. Peszynska, R. E. Showalter

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Outline

1. Introduction

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2. **Model Development**
   - Conservation of mass
   - Solubility constraints
3. **Abstract Evolution Equation**
   - Examples
   - Analysis
4. **Numerical aspects**
   - Fully discrete scheme
   - Semismooth Newton solver

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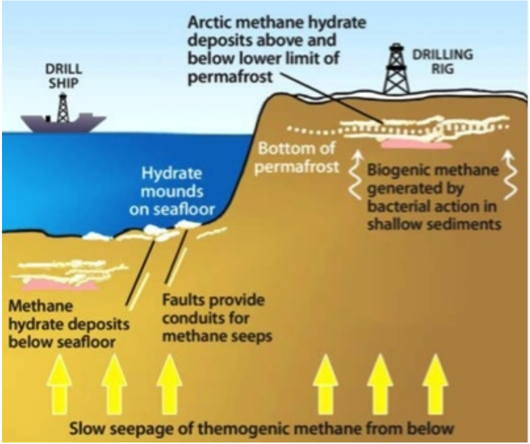

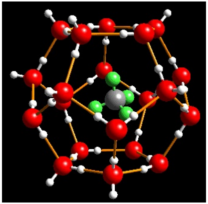

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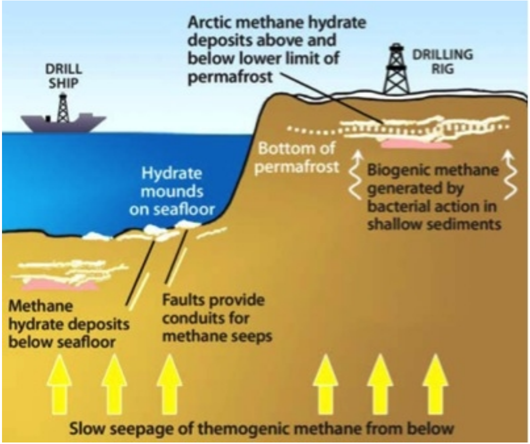

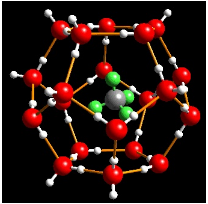

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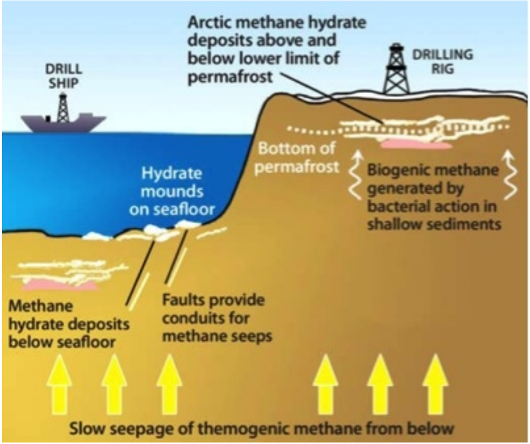

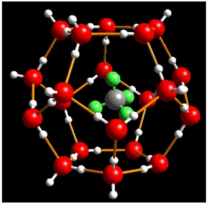

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- We will consider a simplified model of evolution of methane hydrates in the hydrate zone of the sea-bed.
- Components:
  - CH_4
  - H_2O

*[Images from DOE-NETL]

Conservation of mass for CH_4 component

Let $\Omega \subset \mathbb{R}^3$ be a bounded region of points $x \in \Omega$.

Parameters: (assumed given)
ϕ_0 porosity
K_0 permeability
f_M external source of CH_4

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Assumptions:

- Pressure $P(x)$ given by hydrostatic gradients
- Temperature $T(x)$ given by geothermal gradients
- High pressure and low temperature imply Hydrate zone: only liquid and hydrate phases present

Conservation of mass for CH_4 component (cont.)

Unknowns:

- S_l, S_h saturations (void fractions), with $S_h = 1 - S_l$
- $\chi_{lM}, \chi_{lW}, \chi_{lS},$ with $\chi_{lM} + \chi_{lW} + \chi_{lS}, = 1$
  mass fractions of methane, water and salt in liquid phase

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

where densities ρ_l, ρ_h and diffusion D_{lM} are assumed constant.

Unified notation

We redefine parameters

$$R := \frac{\rho_h \chi_{hM}}{\rho_l}, \; f := \frac{f_M}{\rho_l \phi_0}, \; D_0 := \frac{D_{lM}}{\phi_0},$$

and redefine variables

$$S := S_l, \; v := \chi_{lM}, \; u := Sv + R(1 - S),$$

so that (1) becomes

$$\frac{\partial u}{\partial t} - \nabla \cdot (D_0 \nabla v) = f, \tag{2}$$

where we may further scale the problem so that $D_0 = 1$.

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Solubility constraint

$$\begin{cases} \chi_{lM} \leq \chi_{lM}^{\max}, & S_l = 1, \\ \chi_{lM} = \chi_{lM}^{\max}, & S_l \leq 1, \\ (\chi_{lM}^{\max} - \chi_{lM})(1 - S_l) = 0. \end{cases} \tag{3}$$

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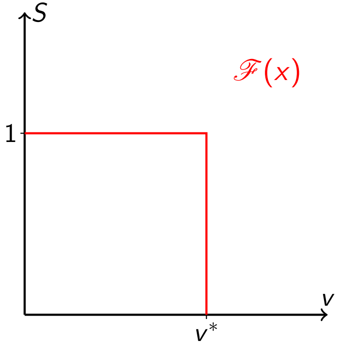

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In our unified notation, we let $v^* = \chi_{IM}^{\max}$, so that

$$\langle v, S \rangle \in \mathscr{F}(x; \cdot) := [0, v^*(x)] \times \{1\} \cup \{v^*(x)\} \times (0, 1]$$

Or equivalently,

$$v \in \alpha_{MH}(x; u) := (u - v^*(x))_- + v^*(x), \; u \le R. \tag{4}$$

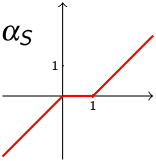
We consider the initial boundary-value problem

Abstract Evolution Equation

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

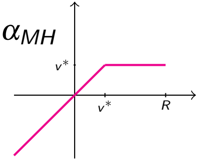
where α is *maximal montone*, or in the case of a measureable family $\{\alpha(x;\cdot) : x \in \Omega\}$, each is a maximal monotone relation.

Examples: $\alpha(u) = \alpha_S, \alpha_{MH}, \underbrace{\alpha_E, \alpha_W}_{\text{Toy models}}, \alpha_{PM}$; $\quad Note : \beta(v) = \alpha^{-1}$



Stefan free-boundary problem:

$$\alpha_S(u) = u_- + (u-1)_+$$



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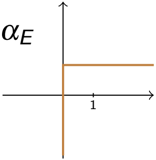
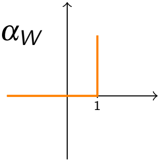


Elbow

Showalter [1984]



Woble

Porous medium equation:

$$\alpha = \alpha_{PM}(u) = |u|u^{m-1}\ (m > 1 \text{ slow diffusion}, \quad 0 < m < 1 \text{ fast diffusion})$$

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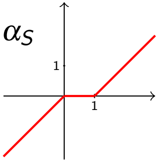

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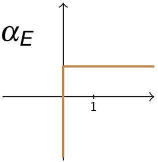

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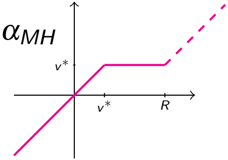

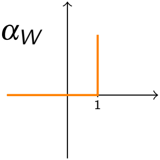

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Summary of theoretical results for α_{MH}

- For the single graph case, we represent the non-linearity as a subgradient, and prove a useful comparison principle, which allows to extend the graph of $\beta = \alpha^{-1}$ to one which is affine bounded. Optimal regularity results follow.
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  - Properties of u, v are the same as those for the Stefan problem.
- We extend existing theory for *porous medium equation* to cover the case of a measureable family of graphs in order to show well-posedness.
  - Based on a normal convex integrand construction.

Details in Gibson, Medina, Peszynska, and Showalter [2013]

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

First, we apply fully implicit time stepping.
Let $\mathscr{V}_h \subset \mathscr{V}$ be the finite element space of continuous piecewise linears on triangulation of Ω.

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

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

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$\mathbf{M}$: mass matrix

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Mass-lumping allows $\mathbf{A_h} = \mathbf{M}^{-1}\mathbf{K}$

Fully discrete scheme

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

where the constraint is applied point-wise.

Lemma [N.Gibson, P. Medina, M. Peszynska, R.E. Showalter]

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

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Corollary

The discrete scheme is uniquely solvable for each of $\beta = \beta_{MH}(x,\cdot), \beta_S, \beta_E, \beta_W$.

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- The method also applies when constraints are parameterized by x.

Nonlinear Complementarity Problem (NCP)

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Similarly,

$$\langle v, u \rangle \in \beta_E \equiv \phi_E(u, v) := \min(u, 1 - v) = 0,$$

$$\langle v, u \rangle \in \beta_W \equiv \phi_W(u, v) := \min(1 - u, v) = 0,$$

$$\langle v, u \rangle \in \beta_S \equiv \phi_S(u, v) := u - v - \max(0, \min(u, 1)) = 0.$$

Semismooth Newton solver

Problem solved at every time step becomes

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

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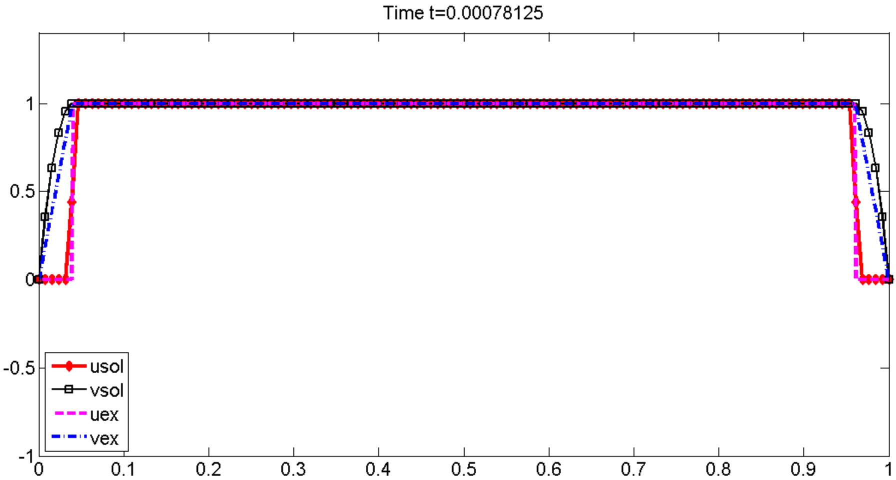
It can be shown that

- each of $\phi_{MH}, \phi_E, \phi_W, \phi_S$ is semi-smooth
- the Jacobian is never singular

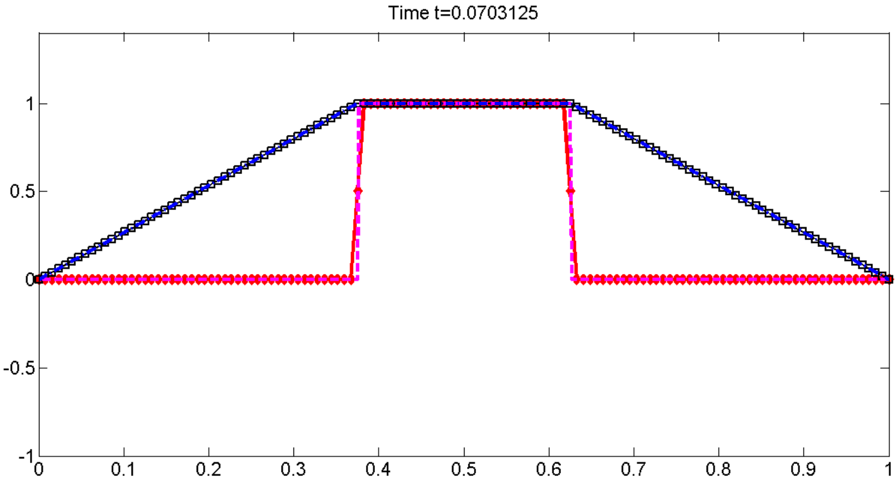
Semismooth Newton converges *superlinearly* for these NCC problems

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

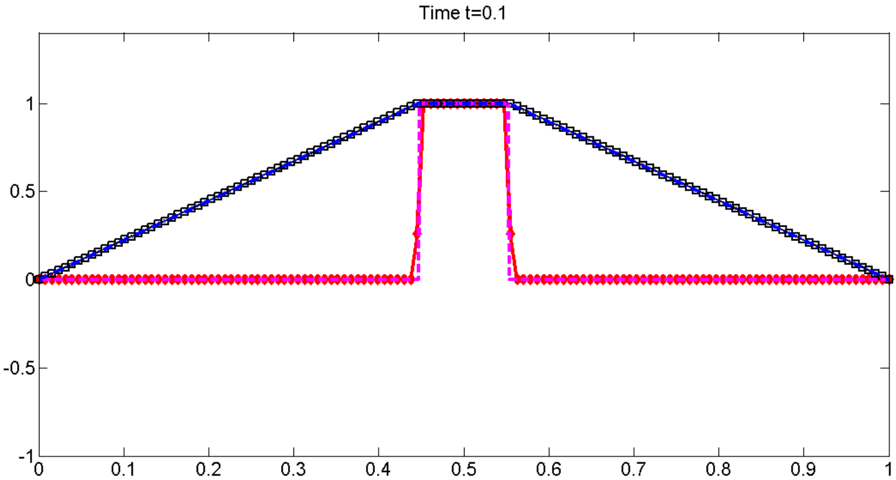
$\alpha = \alpha_E$. Toy model (Showalter [1984]) Frame I



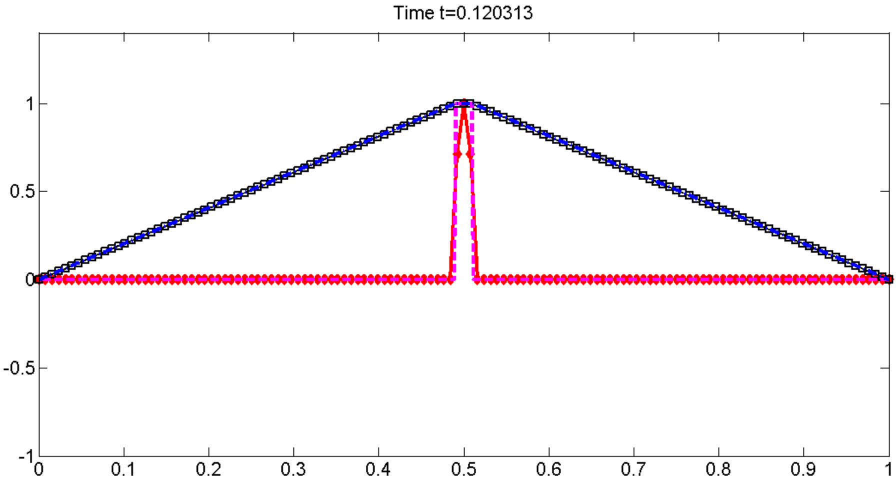
$\alpha = \alpha_E$. Toy model (Showalter [1984]) Frame II



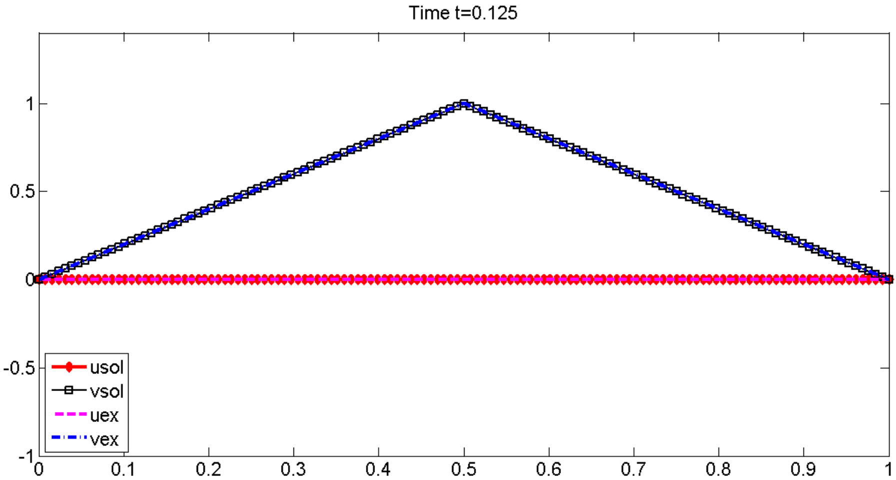
$\alpha = \alpha_E$. Toy model (Showalter [1984]) Frame III



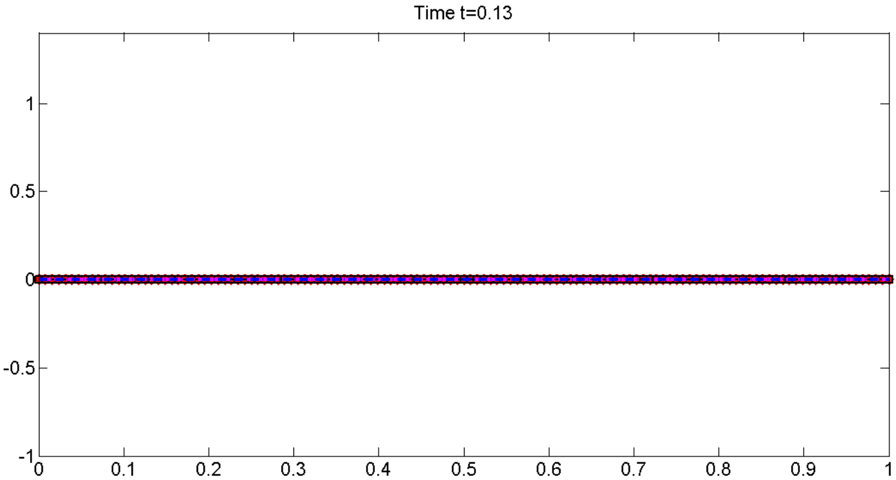
$\alpha = \alpha_E$. Toy model (Showalter [1984]) Frame IV



$\alpha = \alpha_E$. Toy model (Showalter [1984]) Frame V



$\alpha = \alpha_E$. Toy model (Showalter [1984]) Frame VI



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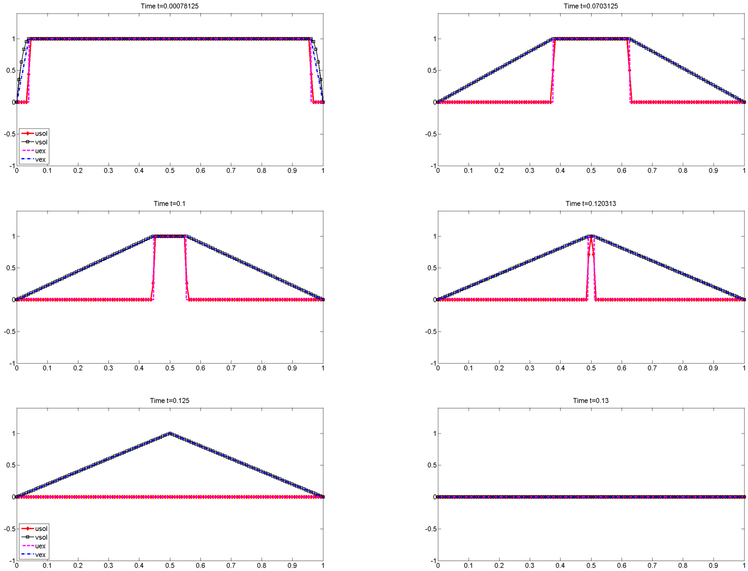


Convergence in u and v for α_E

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

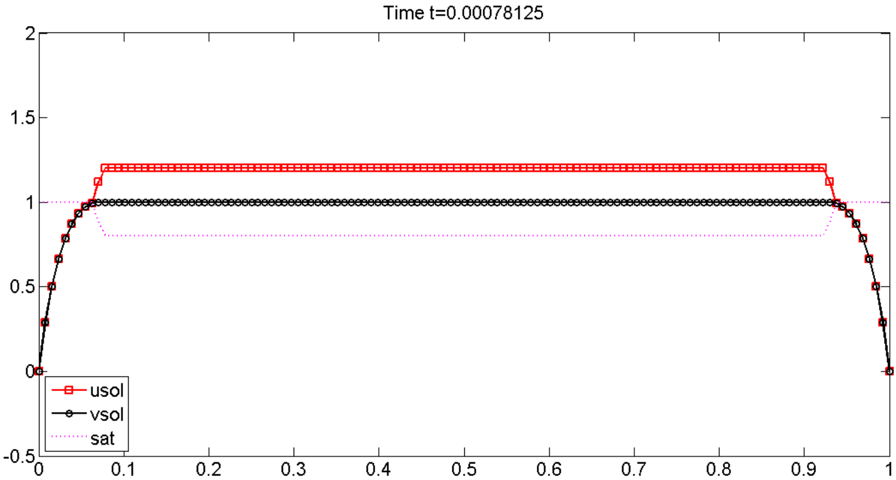
			error	rate	error	rate	error	rate
$1/h$	$1/\tau$	N_{it}	$e_{u,2}$	$r_{u,2}$	$e_{v,2}$	$r_{v,2}$	e_q	r_q
256	2560	2	1.03e-02	0.540	1.19e-03	0.785	6.40e-04	1.073
512	5120	2	6.81e-03	0.601	6.73e-04	0.828	3.00e-04	1.094
128	12800	2	1.47e-02	0.546	1.23e-03	0.966	1.48e-03	1.016
256	25600	2	9.69e-03	0.602	6.29e-04	0.961	7.19e-04	1.040
32	1024	2	2.90e-02	0.516	5.25e-03	0.945	5.42e-03	0.800
64	4096	2	1.93e-02	0.591	2.62e-03	1.003	2.78e-03	0.964

(with quasi-norm: $\sum_n \tau \int_\Omega |u - u_h^n||v - v_h^n| dx$, Ebmeyer and Liu [2008]).

Observed rates

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

$\alpha = \alpha_{MH}$, $v^*_{\max} \equiv 1$. No analytical solution. Frame I



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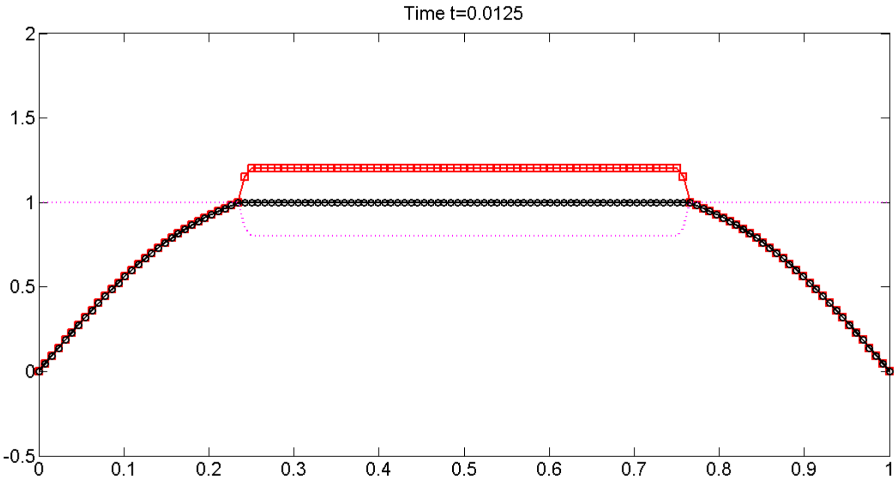

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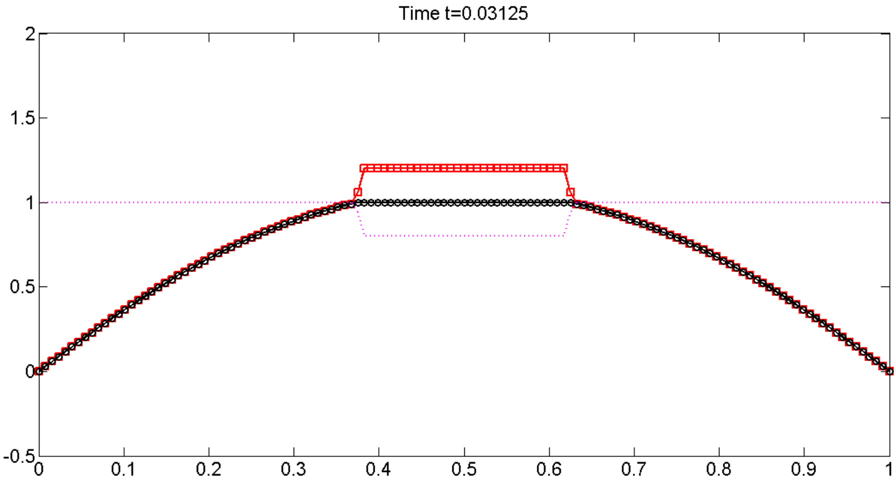

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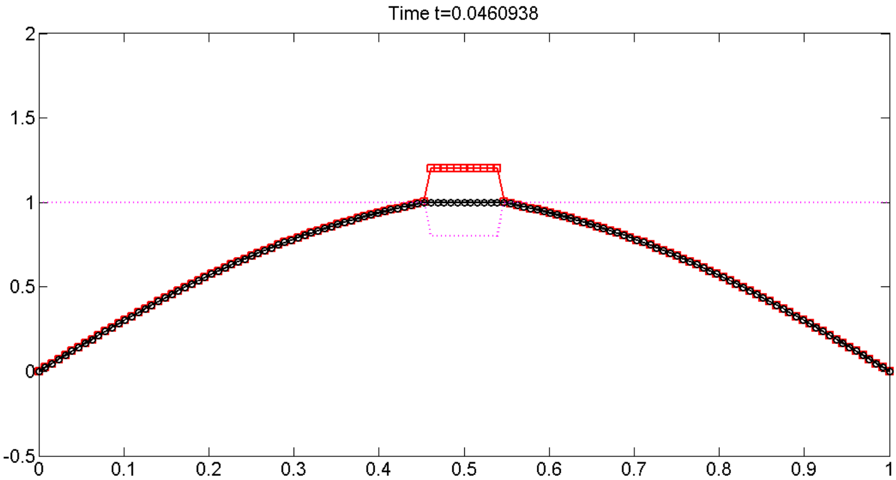
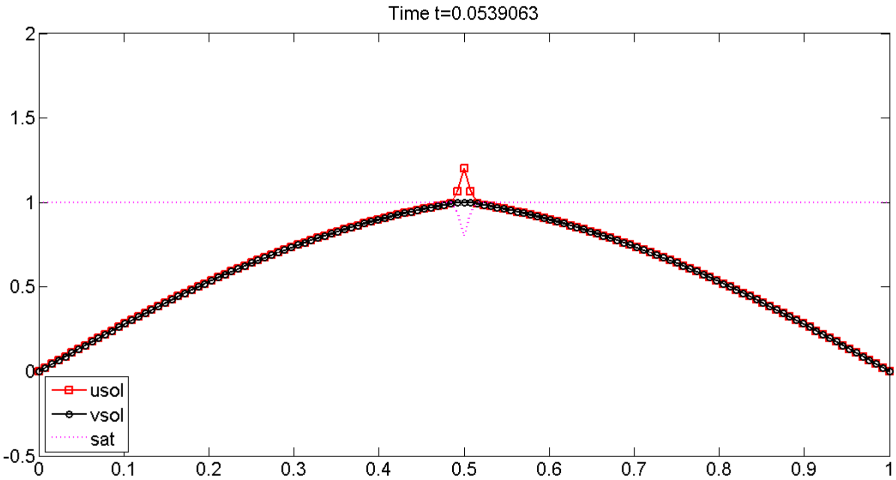


$\alpha = \alpha_{MH}$, $v^*_{\max} \equiv 1$. No analytical solution. Frame V



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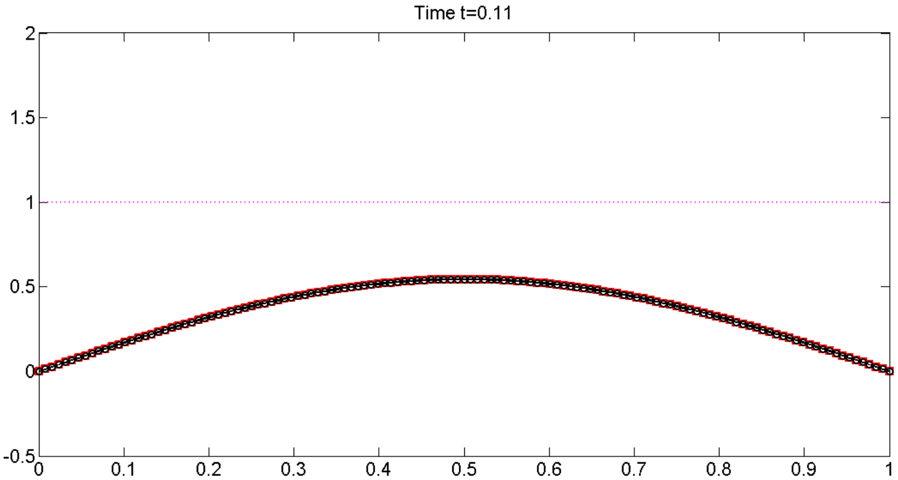

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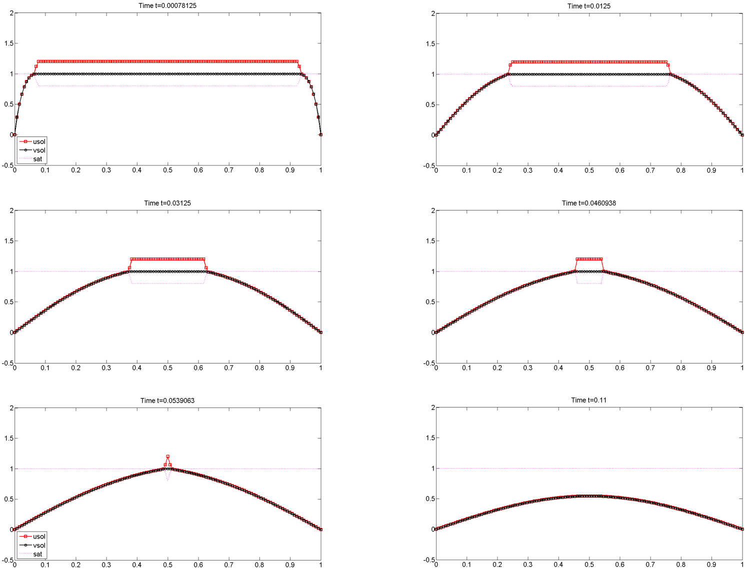


Convergence in u and v for $\alpha_{MH}, v^*_{\max} \equiv 1$.

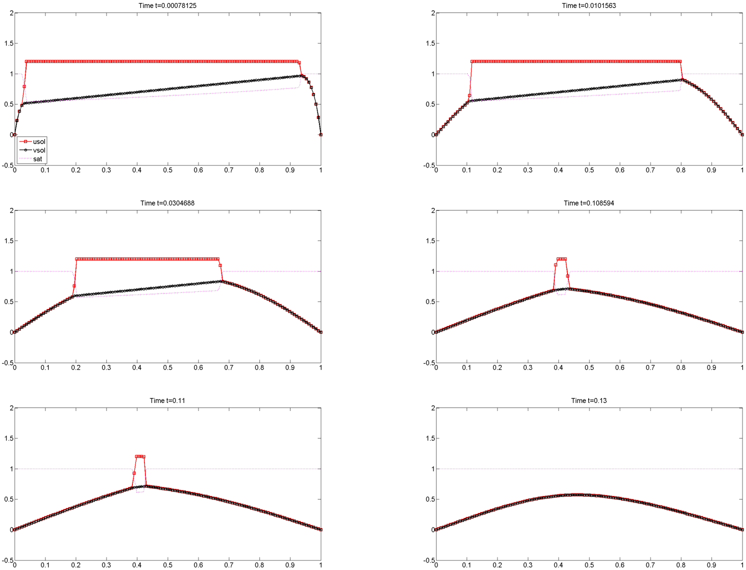
Using $\tau = \frac{h}{10}, \frac{h}{100}, h^2$

$1/h$	$1/\tau$	N_{it}	$e_{u,2}$	$r_{u,2}$	$e_{v,2}$	$r_{v,2}$	e_q	r_q
256	2560	2	2.14e-03	0.560	8.50e-04	0.760	8.62e-04	0.768
512	5120	2	1.39e-03	0.623	4.86e-04	0.806	4.92e-04	0.810
128	12800	2	1.98e-03	0.559	2.17e-04	0.682	3.33e-04	0.855
256	25600	2	1.31e-03	0.603	1.31e-04	0.725	1.81e-04	0.883
32	1024	2	4.39e-03	0.833	1.31e-03	1.396	1.55e-03	1.287
64	4096	2	2.69e-03	0.705	4.88e-04	1.421	6.57e-04	1.239

Observed rates

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

$\alpha = \alpha_{MH}(x;\cdot)$, $v^*_{max}(x) = (1+x)/2$



Convergence rates in u and v for $\alpha = \alpha_{MH}(x;\cdot)$, $v^*_{\max}(x) = (1+x)/2$

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

$1/h$	$1/\tau$	N_{it}	$e_{u,2}$	$r_{u,2}$	$e_{v,2}$	$r_{v,2}$	e_q	r_q
256	2560	2	5.22e-03	0.551	6.74e-04	0.762	7.27e-04	0.798
512	5120	2	3.44e-03	0.602	3.84e-04	0.810	4.07e-04	0.838
128	12800	2	7.11e-03	0.545	2.47e-04	1.039	6.94e-04	0.986
256	25600	2	4.69e-03	0.601	1.29e-04	0.941	3.45e-04	1.010
32	1024	2	1.43e-02	0.622	1.30e-03	1.262	2.57e-03	0.942
64	4096	2	9.35e-03	0.612	5.52e-04	1.236	1.29e-03	0.997

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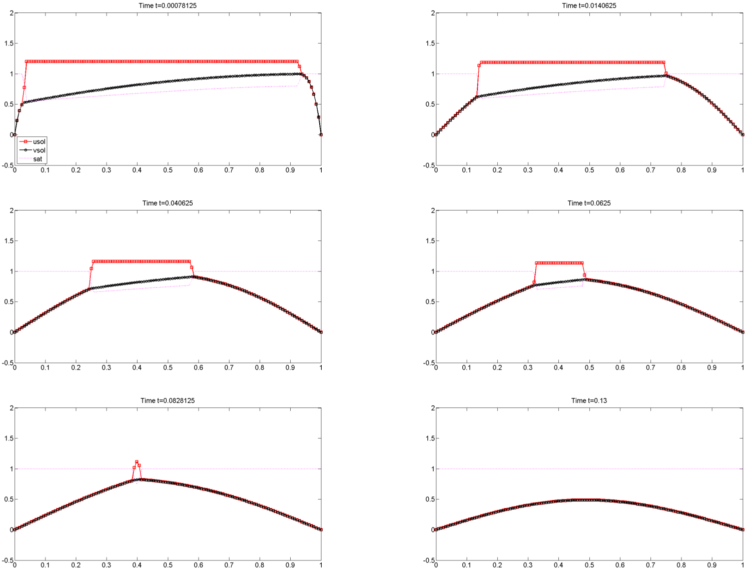

Convergence in u and v for $\alpha = \alpha_{MH}(x;\cdot)$, $v^*_{\max}(x) = (1+2x-x^2)/2$

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

$1/h$	$1/\tau$	N_{it}	$e_{u,2}$	$r_{u,2}$	$e_{v,2}$	$r_{v,2}$	e_q	r_q
256	2560	2	3.45e-03	0.561	6.77e-04	0.763	7.07e-04	0.785
512	5120	2	2.27e-03	0.605	3.86e-04	0.811	3.98e-04	0.827
128	12800	2	4.50e-03	0.554	2.19e-04	0.990	5.33e-04	0.967
256	25600	2	2.96e-03	0.604	1.19e-04	0.875	2.68e-04	0.995
32	1024	2	9.18e-03	0.636	1.18e-03	1.330	1.98e-03	1.013
64	4096	2	5.98e-03	0.619	4.86e-04	1.280	9.88e-04	1.000

Observed rates

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

Convergence in S for $\alpha = \alpha_{MH}$

Using $\tau = \dfrac{h}{100}$

	constant		affine		non-affine	
$1/h$	$e_{S,2}$	$r_{S,2}$	$e_{S,2}$	$r_{S,2}$	$e_{S,2}$	$r_{S,2}$
64	2.91e-03	0.537	7.89e-03	0.519	5.27e-03	0.525
128	1.97e-03	0.559	5.41e-03	0.546	3.58e-03	0.556
256	1.30e-03	0.602	3.56e-03	0.600	2.36e-03	0.603

Observed rates

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

(Similar to rates in u.)

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- Semismooth Newton solver requires mesh independent iterations.
- Convergence rates for examples agree with optimal results for the Stefan problem.
- Incidentally discovered a semismooth Newton method for the Stefan problem.

Future work

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- Semi-implicit time stepping.

References

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