EVOLUTION OF PHASE TRANSITIONS IN METHANE HYDRATE

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Abstract. We consider a simplified model of methane hydrates which we cast as a nonlinear evolution problem. For its well-posedness we extend the existing theory to cover the case in which the problem involves a measurable family of graphs. We represent the nonlinearity as a subgradient and prove a useful comparison principle, thus optimal regularity results follow. For the numerical solution we apply a fully implicit scheme without regularization and use semismooth Newton algorithm for a solver, and the graph is realized as a complementarity constraint (CC). The algorithm is very robust and we extend it to define an easy and superlinearly convergent fully implicit scheme for Stefan problem and other multivalued examples.

KEYWORDS: monotone evolution problems, subgradient, convex normal integrand, semismooth Newton methods, complementarity constraints, methane hydrates, Stefan problem

1. Introduction

In this paper we investigate a model of phase transitions occuring due to solubility constraints during evolution of methane hydrates. We are interested specifically in the formation and dissociation of the hydrate phase out of the methane dissolved in the liquid phase. The treatment of the general multiphase multicomponent model including a gas phase or additional unknowns such as salinity, pressure and temperature is outside the present study.

Our model is a single PDE with two unknowns, the solubility v and saturation S, bound together by an inequality constraint that can be written in the form

$$\frac{\partial u(v,S)}{\partial t} - \triangle v = 0,\ \langle v, S\rangle \in F, \tag{1}$$

where $u(v,S)$ is a function of v and S and $F \subseteq \mathbb{R}^2$ is a multivalued graph. All equations and inclusions such as (1) will be made precise below, holding pointwise almost everywhere on a region or in an appropriate function space.

We transform the model (1) to a form more convenient for analysis

$$\frac{\partial u}{\partial t} - \triangle v = 0,\ v \in \alpha(u)\,, \tag{2}$$

where α is a maximal monotone graph. Formally equivalent to (2) is the formulation in terms of the inverse $\beta \equiv \alpha^{-1}$. The model (2) has been the subject of intense analysis and approximation for the last

four decades. The works summarized in [55] include those for the Stefan free-boundary problem and the porous medium equation.

In a practical methane hydrates model, the graph F is parametrized by several independent and dependent variables other than S, v, u. In the simplest variant F is strongly dependent on the depth of the reservoir Ω, i.e., on the position variable $x \in \Omega$,

$$\langle v, S \rangle \in F(x). \tag{3}$$

In the transformed model, the variables u and v are related by a monotone graph relationship dependent on x,

$$\frac{\partial u}{\partial t} - \triangle v = 0, \ v \in \alpha(x; u). \tag{4}$$

This additional parametrization is smooth in x but its analysis requires an extension of standard theory for the porous medium equation. This is the main theoretical contribution here. Our analysis of (4) supplemented by appropriate boundary and initial conditions is based on a normal convex integrand construction extending the theory for the porous medium equation.

Next we take advantage of the physical meaning of F being a *solubility constraint* and rewrite it as a *nonlinear complementarity constraint* (NCC). Here we follow the ideas in [23] which were recommended to us by Peter Knabner [29]. While (4) is *not* merely a variational parabolic inequality, we can still draw on the techniques that have recently become successful in solving the latter numerically. In particular, we take advantage of the framework of semi-smooth Newton methods [54, 24] for solving the discrete nonlinear problems under NCCs. To this aim, we formulate a fully discrete numerical model for (4) and we rewrite (3) as

$$\phi(x; v, S) = 0, \tag{5}$$

where ϕ is some *semismooth* function [54] that is chosen appropriately corresponding to the given α. The algebraic problem can be solved by a semismooth Newton method, and we have thereby resolved a possibly singular graph relationship *without* regularization.

In fact, we can solve our problem in either (v, S) or in (v, u) formulations with convergence properties not worse than those for the Stefan problem, while exploiting the ease and superlinear convergence of the semismooth Newton methods. This is an important practical contribution. Furthermore, we show that our algorithm is formally equivalent to the *variable switching* method used in engineering

implementations of models similar to (4) [22, 41, 13] and in particular for methane hydrates [33] which has not been analyzed.

The semismooth solver is in fact so robust that we test it on some multivalued examples. In addition, we propose an appropriate ϕ for the Stefan problem using *box constraints*, and so its fully implicit solution *without regularization* is very easy with a small mesh-independent number of iterations. This is an improvement over regularized and relaxation-based solvers [38, 36, 3, 56].

Throughout the paper we adopt the following notation with which we distinguish pairs $\langle u, v\rangle \in f \subset \mathbb{R}^2$ from the usual Cartesian coordinates $(x, y) \in \Omega \subset \mathbb{R}^2$. The relation symbol $\langle u, v\rangle$ is also used in the setting when $u, v \in \mathcal{H}$ and $\mathcal{H}$ is a Hilbert space. Furthermore, if f is a relation, we denote that $\langle u, v\rangle \in f$ by writing $v \in f(u)$, and this emphasizes that f can be regarded as a set-valued function. If $f \subset \mathbb{R}^2$ is a function in the usual sense, we write instead $v = f(u)$, but we still identify f with its graph. If $\langle u, v\rangle \in f$, we define the inverse relation f^{-1} naturally by $\langle v, u\rangle \in f^{-1}$; then f^{-1} is a set-valued function as well. For example, the Heaviside graph is described by

$$H \equiv \{\langle x, y\rangle \in \mathbb{R}^2 : 0 \le y \le 1,\ yx \ge 0,\ (y-1)x \ge 0\}. \tag{6}$$

If a graph f is dependent on a parameter x, we denote this by $v \in f(x; u)$, and $\langle u, v\rangle \in f(x; \cdot)$, etc.

This paper is organized as follows. In Section 2 we develop the model and cast it in the form (4). We analyze its well-posedness in Section 3 where particular attention is paid to the construction of an appropriate normal convex integrand whose subgradient is the inverse $\beta(x; \cdot) = \alpha(x; \cdot)^{-1}$. In addition, we demonstrate a comparison principle which lets us extend the graph β to one which is affine bounded on all of $\mathbb{R}$, and this helps to establish regularity of solutions. In Section 4 we discuss the discrete scheme and prove some of its properties, as well as introduce the framework of semismooth Newton methods. Numerical results are shown in Section 5.

2. Model development

Methane hydrates are an ice-like substance containing methane molecules trapped in a lattice of water molecules. They are present in large amounts along continental slopes and in permafrost regions, and modeling of their evolution is important, since the hydrates of methane and carbon dioxide play important roles as both potential energy sources and environmental hazards [18, 53]. Here we consider a simplified model of evolution of methane hydrates in the hydrate zone of the sea-bed. See [33, 40, 39] for full model including the energy equation with latent heat, and multiple components in the presence of multiple phases.

Let $\Omega \subset \mathbb{R}^d, d = 1, 2, 3$, be a bounded region of points $x \in \Omega$. The properties of the sediment which fills the region Ω are its porosity ϕ_0 and permeability K_0. For simplicity of the exposition we consider these constant, but in general it is straighforward to extend the results below to the heterogeneous case $\phi_0(x), K_0(x)$. In particular, it is generally true that both $\phi_0(x), K_0(x)$ decrease with depth. Next, let $P(x)$ and $\theta(x)$ denote the pressure and temperature in the reservoir, respectively. We assume these are known and given by hydrostatic and geothermal gradients, respectively. In particular we note that both $P(x)$ and $\theta(x)$ increase with depth. This is a common characteristic of sea sediment hydrates [33].

We assume the pressure is high enough and temperature is low enough in Ω so that only the liquid and hydrate phases can be present. The presence of these two phases is accounted for by their saturations, i.e., void fractions, S_l, S_h, respectively. Since $S_l + S_h \equiv 1$, only one of these phase saturations is an independent variable. We choose here the dominant liquid phase saturation and denote it by $S \equiv S_l$. The two phases have respective densities ρ_l, ρ_h which are mildly dependent on the pressures and temperature. The liquid phase consists of water, salt, and methane components, and their corresponding mass fractions are denoted by $\chi_{lW}, \chi_{lS}, \chi_{lM}$, respectively. The hydrate phase is made of molecules of water and of methane, with the mass fractions denoted by χ_{hW}, χ_{hM}. Because of the physical nature of hydrate crystals which usually are built from a fixed proportion of methane and water molecules, it is common to assume the last two are constants, while $\chi_{lW}, \chi_{lS}, \chi_{lM}$ are variables. In this paper we will assume that χ_{lS} is known and fixed, with a value equal to that of seawater. Since for mass fractions in the same phase we have $\chi_{lW} + \chi_{lS} + \chi_{lM} \equiv 1$ [[31], *(2.2.8a)*], only one of the variables χ_{lW}, χ_{lM} is independent, and we choose methane solubility χ_{lM} as the independent variable.

Under these assumptions, we only model the evolution of χ_{lM} and of S_l. The equations governing these variables come from (i) the conservation of mass of methane, and from (ii) thermodynamics. Furthermore, hydrostatic equilibrium is assumed here, so there is no flow of water phase and the evolution of methane follows only via diffusion of methane molecules in the liquid phase. The coefficient D_{lM} may be dependent upon other quantities, but in this paper we assume it is constant. The conservation of mass for the methane component takes the form

$$\frac{\partial}{\partial t}(\phi_0 S_l \rho_l \chi_{lM} + \phi_0 S_h \rho_h \chi_{hM}) - \nabla \cdot (D_{lM} \rho_l \nabla \chi_{lM}) \quad = \quad f_M. \tag{7}$$

In this equation f_M is an external source of methane, e.g., due to bacteria–induced methanogenesis. Furthermore,

$$N_M := S_l \rho_l \chi_{lM} + S_h \rho_h \chi_{hM} = S_l \rho_l \chi_{lM} + (1 - S_l) \rho_h \chi_{hM} \tag{8}$$

is the total mass of methane per unit volume; N_M accounts for the methane present both in the liquid and hydrate phases. In summary, note that all the coefficients of (7) are given as data, and the only independent variables are χ_{lM}, S_l. To complete the model, we need to tie these two unknowns χ_{lM}, S_l together. This is done consistent with the Gibbs phase rule [31] via thermodynamics of solubility constraints.

2.1. **Solubility constraints.** The amount of methane that can be dissolved in the liquid phase depends on the pressure P_l, temperature θ, and the salinity χ_{lS}. Conversely, these variables determine under what circumstances $S_l < 1$, i.e., when the hydrate phase can be present. In the hydrate literature [33, 52] the data for the *maximum solubility constraint* χ_{lM}^{max} is provided as a function of P, θ, χ_{lS}. Here we assume these variables are known functions of x so this provides us with $\chi_{lM}^{max} = \chi_{lM}^{max}(x)$. Typically, χ_{lM}^{max} increases with depth within the hydrate zone; see [53, 33, 40]. Since we must have $\chi_{lM}(x,t) \le \chi_{lM}^{max}(x)$ at any $(x,t) \in \bar{Q}$, the quantity χ_{lM}^{max} determines how the total amount of methane N_M is partitioned between the liquid and hydrate phases. If $\chi_{lM}(x,t) < \chi_{lM}^{max}(x)$, then only the liquid phase is present, i.e., $S_l(x,t) = 1$. Then $N_M = \rho_l \chi_{lM}$ and χ_{lM} determines the amount of methane and is the independent variable. On the other hand, when the amount present reaches the maximum amount that can be dissolved, i.e., $N_M = \rho_l \chi_{lM}^{max}$, the excess forms the hydrate phase with $S_h = 1 - S_l > 0$. In this case S_l becomes the independent variable while $\chi_{lM}(x,t) = \chi_{lM}^{max}(x)$ is fixed.

We express this process as was done succintly in [23] for a hydrogen model as

$$\begin{cases} \chi_{lM} \le \chi_{lM}^{max}, & S_l = 1\,, \\ \chi_{lM} = \chi_{lM}^{max}, & S_l \le 1\,, \\ (\chi_{lM}^{max} - \chi_{lM})(1 - S_l) & = 0\,. \end{cases} \tag{9}$$

This form shows that the solubility satisfies a nonlinear complementarity constraint (NCC). Our numerical algorithm discussed in the sequel takes advantage of this form of the constraint. For analysis, it is more convenient to write the constraint (9) as a multivalued graph

$$\langle \chi_{lM}, S_l \rangle \in \mathcal{F}_x := [0, \chi_{lM}^{max}] \times \{1\} \cup \{\chi_{lM}^{max}\} \times (0, 1]. \tag{10}$$

Note that since χ_{lM}^{max} depends on x, the graph $\mathcal{F}_x$ is parametrized by x as well.

Remark 2.1. *Strictly speaking, the graph* (10) *is only a subgraph of*

$$\langle \chi_{lM}, S_l \rangle \in \mathcal{F}_\infty := (-\infty, \chi_{lM}^{max}] \times \{1\} \cup \{\chi_{lM}^{max}\} \times (-\infty, 1], \tag{11}$$

truly equivalent to the NCC in (9). *Throughout this paper we will assume that*

$$S_l \geq 0, \chi_{lM} \geq 0 \tag{12}$$

which turns (11) *into* (10). *While* (12) *is required on physical grounds, it is not enforced in our model as an additional constraint but rather follows as a consequence of the maximum principle. (See Corollary 3.2.)*

For the sake of exposition, we further simplify (7) and assume that

$$\rho_l \approx const,\ \rho_h \approx const,\ \phi_0 \approx const,\ D_{lM} = const. \tag{13}$$

The simplifying assumptions let us further rewrite (7), upon algebraic manipulations, as

$$\frac{\partial}{\partial t}(S_l\chi_{lM} + R(1 - S_l)) - \nabla \cdot (D_0 \nabla \chi_{lM}) = f \tag{14}$$

where we have defined $R := \frac{\rho_h \chi_{hM}}{\rho_l}$, $f := \frac{f_M}{\rho_l \phi_0}$, $D_0 = \frac{D_{lM}}{\phi_0}$.

2.2. **Summary of the model with simplified notation.** To avoid multiple subscripts, in the rest of the paper we introduce the variables $S = S_l, u = \frac{N_M}{\rho_l}, v = \chi_{lM}, v^* = \chi_{lM}^{max}$. We rewrite the model comprised of the partial differential equation (14) and constraint (9) as

$$\frac{\partial u}{\partial t} - \nabla \cdot (D_0 \nabla v) = f,\ u := Sv + R(1 - S), \tag{15a}$$

$$\langle v, S\rangle \in \mathcal{F}(x; \cdot) := [0, v^*(x)] \times \{1\} \cup \{v^*(x)\} \times (0, 1]. \tag{15b}$$

We will assume henceforth that

$$v^* \quad : \quad \Omega \to \mathbb{R} \text{ is (at least) piecewise smooth,} \tag{16}$$

$$\min_{x\in\Omega}(v^*(x)) \quad \geq \quad v_0 > 0, \text{ and} \tag{17}$$

$$R \quad > \quad \max_{x\in\Omega}(v^*(x)). \tag{18}$$

These assumptions are physically grounded. The diffusivity and maximum solubilities are always non-negative, while (18) follows from thermodynamics and is true for available data, e.g., in [33, 52] that we used in [40].

It is useful to derive an explicit relationship between u and v, and u and S. It is not hard to see that

$$\langle v, u\rangle \in \beta_{MH}(x; \cdot) := \{(v, v) : v \leq v^*(x)\} \cup \{v^*(x)\} \times [v^*(x), R) \tag{19}$$

The inverse of this relation for each $x \in \Omega$,

$$v = \alpha_{MH}(x;u) = (u - v^*(x))_- + v^*(x), \quad u \le R, \tag{20}$$

is a monotone Lipschitz function. We denote by $u_- = \min(u, 0)$ the negative part of u. The constant D_0 can be included in the definition of α, so we set $D_0 = 1$.

Remark 2.2. *For each fixed x both $\alpha_{MH}(x;\cdot)$ and $\beta_{MH}(x;\cdot)$ are monotone graphs.*

Finally, $S = S(x;u)$ is a function

$$S = \frac{u-R}{v-R} = \begin{cases} 1, & u \le v^*(x), \\ \frac{u-R}{v^*(x)-R}, & u > v^*(x), \end{cases} \tag{21}$$

which by (18) is monotone decreasing in u, with values in $[0,1]$ as long as $0 \le u \le R$.

The model (15) is a nonlinear evolution problem which must be complemented by initial conditions on u and boundary conditions in v. Its well-posedness and numerical approximation are discussed in the sequel.

3. Analysis of PDE with parameter dependent family of graphs

We consider here the initial-boundary-value problem

$$\frac{\partial u}{\partial t} - \Delta v = f, \quad v \in \alpha(\cdot;u) \text{ on } \Omega \times (0,T), \tag{22a}$$

$$v = 0 \text{ on } \partial\Omega \times (0,T), \tag{22b}$$

$$u(\cdot,0) = u_0(\cdot) \text{ on } \Omega, \tag{22c}$$

to be satisfied in an appropriate weak sense. Boundary conditions on $\partial\Omega$ other than homogeneous Dirichlet type are needed for practical problems but for simplicity are not considered here. Our analysis of (22) proceeds as follows. In Section 3.1 we review what is known about the special case corresponding to $v^*(x) = const$, in which α is a single monotone Lipschitz function onto $\mathbb{R}$ and $\beta = \alpha^{-1}$ is an affine-bounded graph. Next we develop in Section 3.2 the well-posedness for the x-dependent case $\alpha(x;u)$ corresponding to a spatially dependent constraint $v^*(x)$.

Let $\mathcal{H} = L^2(\Omega)$ denote the usual Lebesgue space with the scalar product $(\cdot,\cdot)$, and let $\mathcal{V} = H_0^1(\Omega)$ be the indicated Sobolev space with the scalar product $(v,w)_{\mathcal{V}} = (\nabla v, \nabla w)$. Its dual space is $\mathcal{V}' = H^{-1}(\Omega)$, and the Riesz map is given by $-\Delta : \mathcal{V} \to \mathcal{V}'$. Note that $\mathcal{V} \subset \mathcal{H} \subset \mathcal{V}'$ and

$$(f,g)_{\mathcal{V}'} = ((-\Delta)^{-1}f, (-\Delta)^{-1}g)_{\mathcal{V}} = f((-\Delta)^{-1}g), \ f,g \in \mathcal{V}'. \tag{23}$$

An equation "on Ω" (or "on $\Omega \times (0,T)$") means that it holds in $\mathcal{V}'$ or $L^1(\Omega)$, (respectively, for a.e. $t \in (0,T)$), and similarly for $\partial\Omega$ and $\partial\Omega \times (0,T)$.

3.1. **Evolution equation with a single monotone graph.** We recall some classical results on the Dirichlet initial-boundary-value problem

$$\frac{\partial u}{\partial t} - \Delta v = f, \quad v \in \alpha(u) \text{ on } \Omega \times (0,T), \tag{24a}$$

$$v = 0 \text{ on } \partial\Omega \times (0,T), \tag{24b}$$

$$u(\cdot,0) = u_0(\cdot) \text{ on } \Omega. \tag{24c}$$

This can be formulated as an abstract initial-value problem

$$\frac{du(t)}{dt} + A(u(t)) \ni f(t) \text{ a.e. on } (0,T], \quad u(0) = u_0, \tag{25}$$

in a Banach or Hilbert space setting with

$$A = -\triangle \circ \alpha \tag{26}$$

on the appropriate domain $D(A)$. There are two notions of solution:

$$u \in C([0,T], L^1(\Omega)) \text{ with } v(t) \in W_0^{1,1}(\Omega),\ \Delta v(t) \in L^1(\Omega), \tag{27}$$

$$u \in W^{1,1}([0,T], \mathcal{V}') \text{ with } v(t) \in \mathcal{V}. \tag{28}$$

These follow since the operator A is m-accretive on the Banach space $L^1(\Omega)$ and on the Hilbert space $\mathcal{V}'$, respectively. If the initial value $u_0 \in L^1(\Omega) \cap \mathcal{V}'$, our solution satisfies both [50].

3.1.1. *Examples.* In addition to our problem in which $\alpha(\cdot) = \alpha_{MH}(x;\cdot)$ is given by (20), classical examples of (24) include the porous medium equation in which $\alpha = \alpha_1(u) = |u|u^{m-1}$, with $m > 1$ for slow diffusion and $0 < m < 1$ for fast diffusion. The Stefan free-boundary problem has

$$\alpha_{ST}(u) = u_- + (u-1)_+\,, \tag{29}$$

where $u_+ = \max(u,0)$ and $u_- = \min(u,0)$ are the positive and negative parts of u. The examples

$$\alpha_E = \{0\} \times (-\infty, 1] \cup [0,\infty) \times \{1\} \text{ and} \tag{30}$$

$$\alpha_W = \alpha_E^{-1} = (-\infty, 1] \times \{0\} \cup \{1\} \times [0,\infty) \tag{31}$$

from [50] are included below. These are the limits of the fast and slow diffusion, respectively, as $m \to 0$, and $m \to \infty$.

Remark 3.1. *For slow and fast diffusion α is a monotone continuous function from $\mathbb{R}$ onto $\mathbb{R}$, but $\alpha,\ \beta$ are not Lipschitz at 0 for the fast, slow diffusion cases, respectively. For the Stefan problem* (29) *the graph α_{ST} is a maximal monotone Lipschitz continuous function that is affine bounded and onto $\mathbb{R}$. The graph α_E in* (30) *and its inverse are each maximal monotone, but neither is a function. For the methane hydrate problem the graph $\alpha_{MH}(x;\cdot)$ given by* (20) *is Lipschitz continuous and monotone but not maximal, and its range is a proper subset of $\mathbb{R}$. For constant v^* it is easily extended as a translate of the Stefan graph* (29)*.*

Known results for (24) require that α be maximal monotone. (See [55, 57], [[51], *p234*].) For the case (20) we shall extend the graph beyond the given domain to a graph that is maximal, so the well-posedness theory may be applied. The *maximum principle* for (24) from [7] that shows that, with compatible data, the solution does not go outside known bounds. Thus we can alter the definition of α at values outside the range of values of the (bounded) solution.

Regularity results stronger than (28) are obtained in the Hilbert space setting with a subgradient type operator (see below). In particular, the estimates of [[57], *II.5.1*] provide $L^2(\Omega \times (0,T))$ results for v; these require an affine growth bound on both $\alpha,\ \beta$. In particular, if α is Lipschitz and monotone then $u \in L^2(\Omega \times (0,T])$ [[57], *II.3.1*] or [[26], *5.2*].

Background for abstract setting. We recall some background material to be used in Section 3.2. An operator A on a Banach space B is a relation $A \subset B \times B$ with (possibly multiple) values $A(x) = \{y \in B : \langle x, y\rangle \in A\}$ at each $x \in Dom(A)$, the domain of A. A is *accretive* on B if for each $\langle x_1, y_1\rangle, \langle x_2, y_2\rangle \in A$ and $\varepsilon > 0$ we have $\|x_1 - x_2\| \le \|x_1 + \varepsilon y_1 - (x_2 + \varepsilon y_2)\|$. It is *m-accretive* if also the range $Rg(I + A) = B$. In a Hilbert space H with scalar product $(\cdot,\cdot)_H$, A is *accretive* if $(y_1 - y_2, x_1 - x_2)_H \ge 0$ for $\langle x_1, y_1\rangle, \langle x_2, y_2\rangle \in A$. These are also called *monotone* and *maximal monotone*, respectively.

The following result due to T. Kato is well known for the initial-value problem (25); see Corollary 8.4 p. 228 and Thm 4.3 on p. 186, pp. 203-204 of [51].

Theorem 3.1. *Assume A is m-accretive on the Hilbert space H. For each $u_0 \in Dom(A)$ and $f \in W^{1,1}((0,T),H)$, there is a unique $u \in W^{1,\infty}((0,T),H)$ which satisfies* (25)*.*

If A is a *subgradient*, there are additional regularity properties. Let the extended real numbers be denoted by $\mathbb{R}_\infty \equiv \mathbb{R} \cup \{+\infty\}$. Assume the function $\Psi : H \to \mathbb{R}_\infty$ is proper, convex and lower-semicontinuous. Denote by $f \in \partial\Psi(u)$ (equivalently, $\langle u, f\rangle \in \partial\Psi$) that $(f, w - u)_H \le \Psi(w) - \Psi(u)$ for

all $w \in H$. Then the operator $\partial\Psi$ is the *subgradient* of Ψ, and $\partial\Psi : H \to H$ is m-accretive. We have the following theorem due to H. Brezis [[5], *Thm 3.6*].

Theorem 3.2. *Assume $A = \partial\Psi$ is a subgradient on the Hilbert space H, $u_0 \in \overline{Dom(A)}$ and $f \in L^2((0,T),H)$. Then there is a unique $u \in C([0,T],H)$ with $\sqrt{t}\frac{du}{dt} \in L^2((0,T),H)$ and $u(t) \in Dom(A)$ a.e. which satisfies* (25)*. If $u_0 \in Dom(A)$, then $\frac{du}{dt} \in L^2([0,T],H)$.*

Application of abstract setting. In the Hilbert space $H = \mathcal{V}'$ denote by $A = -\Delta \circ \alpha$ the operator with the domain $Dom(A) = \{u \in \mathcal{V}' \cap L^1(\Omega) : \text{for some } v \in \mathcal{V},\ v \in \alpha(u)\}$ and $-\Delta v \in A(u)$ for all such v. With this choice of A, the initial-boundary-value problem (24) is realized as the abstract initial-value problem (25). Theorem 3.2 is known to apply if

$$\alpha(\cdot) \text{ is a maximal monotone graph onto } \mathbb{R}. \tag{32}$$

Then the operator A described above is a *subgradient* in $\mathcal{V}'$ and Theorem 3.2 applies to show well-posedness of (24). See [4, 48], and [[1], *p.206*] or [[51], *p.142-144,203-204*]. Additionally, if α satisfies (32), and $\alpha^{-1}(\cdot)$ has affine growth, an H^{-1} solution is obtained in [17] even in a *doubly-nonlinear* case with $-\Delta$ replaced with a general quasi-linear elliptic operator.

Remark 3.2. *For the Stefan problem α is given by* (29)*, so* (32) *is satisfied and in addition α is Lipschitz continuous on $\mathbb{R}$; see [*[6]*, p35], [*[32]*, Chapter III],* [49]*, or* [51]*A.1. It is known that* (24) *has a unique bounded solution with $\nabla v,\ v_t \in L^2(\Omega \times (0,T))$. See* [2, 6, 4, 10, 17, 51, 30]*. Furthermore, the continuity of $v(x,t)$ was established in* [14, 59, 9, 46, 47, 30]*. If not α but α^{-1} satisfies* (32) *and is Lipschitz, then continuity of $u(x,t)$ follows* [15, 16]*.*

Remark 3.3. *For α given in* (30)*, in order for* (32) *to hold, one needs first to establish a maximum principle to hold which allows the use of an affine-bounded modification of α onto $\mathbb{R}$. Since neither α nor α^{-1} is a function, no additional regularity results are available. This was demonstrated in* [50]*, and an exact and numerical solutions are further discussed in Section 4.*

Remark 3.4. *For α given by* (20)*, the case of primary interest here, we extend the graph α to one that is a translate of Stefan-type graph and conclude that the properties of u, v are the same as those for the Stefan problem.*

3.2. **Evolution equation with a measurable family of graphs.** Our primary objective here is to extend the existence results recalled in Section 3.1 to the initial-boundary-value problem (22) with a measurable family $\{\alpha(x;\cdot) : x \in \Omega\}$ of maximal monotone relations. First we provide the construction

of the family $\alpha(x;\cdot)$ such that for each $x \in \Omega$ the inverse $\beta(x;\cdot)$ is the subgradient of a prescribed convex function $\varphi(x;\cdot)$ on $\mathbb{R}$. The solution to (22) is then analyzed in that framework, and we shall need to demonstrate that $\beta(x;\cdot) - \Delta$ is onto $\mathcal{V}'$. We close the section by formulating and proving a comparison principle for (22).

Measurable family of convex functions. Recall that in Section 3.1 we took advantage of additional regularity of solutions to (25) arising from the fact that $A = -\Delta \circ \alpha$ was a subgradient. For the more general case that $\alpha = \alpha(x;\cdot)$ is parametrized by x, we shall show that A is m-accretive on $\mathcal{V}'$. To do this, we shall exploit the fact that $\beta(x;\cdot) = \alpha^{-1}(x;\cdot)$ is a subgradient on $\mathcal{H}$.

For our application, take $\varphi(x;v) = \frac{1}{2}v^2 + (R - v^*(x))(v - v^*(x))_+$. Then for each $x \in \Omega$ $\beta(x;\cdot) = \partial\varphi(x;\cdot)$ is a maximal monotone extension of (19).

We require the construction of a *normal convex integrand* $\varphi(x;\xi)$ [42, 43, 20]. Thus, we assume

- for each $x \in \Omega$, the function $\varphi(x;\cdot) : \mathbb{R} \to \mathbb{R}_\infty$ is proper, lower semicontinuous and convex,
- for each $\xi \in \mathbb{R}$, the function $x \mapsto \varphi(x;\xi)$ is measurable,
- there is a countable collection B of measurable functions $w : \Omega \to \mathbb{R}$ for which $x \mapsto \varphi(x;w(x))$ is measurable for each $w \in B$, and
- $B(x) \equiv \{w(x) : w \in B\}$ satisfies $B(x) \cap Dom(\varphi(x;\cdot))$ is dense in $Dom(\varphi(x;\cdot))$ for each $x \in \Omega$,

where $Dom(\varphi(x;\cdot)) = \{\xi \in \mathbb{R} : \varphi(x;\xi) < \infty\}$ is the *effective domain.* Since $v^*(x)$ is piecewise smooth, the function $\varphi(x;\cdot)$ has these properties, and the collection B can be constructed from a class of step functions w with rational values.

These conditions guarantee that $x \mapsto \varphi(x;w(x))$ is measurable for each $w \in \mathcal{H}$, not just for those $w \in B$, so we can define the proper, lower semicontinuous and convex function $\Phi : \mathcal{H} \to \mathbb{R}_\infty$ by

$$\Phi(w) = \int_\Omega \varphi(x;w(x))\,dx, \ \ w \in \mathcal{H}. \tag{33}$$

With the subgradient of $\varphi(x;\cdot)$ denoted by $\partial\varphi(x;\cdot)$, the subgradient of $\Phi(\cdot)$ is given (pointwise a.e.) by $\partial\Phi(v)(x) = \partial\varphi(x;v(x))$; that is,

$$u \in \partial\Phi(v) \text{ is equivalent to } u, v \in \mathcal{H}, \text{ and } u(x) \in \partial\varphi(x;v(x)) \equiv \beta(x;v(x)) \text{ a.e. on } \Omega. \tag{34}$$

In fact, it is easy to check that $I + \partial\Phi$ is an extension of $I + \partial\phi(x;\cdot)$ and that the latter operator is onto $\mathcal{H}$, so it follows that these are equal. The inverse $(\partial\Phi)^{-1}$ is likewise maximal monotone on $\mathcal{H}$.

Abstract formulation with $\partial\Phi$. The initial-boundary-value problem (22) will be formulated as (25) in $\mathcal{V}'$. Define the operator A on $\mathcal{V}'$ by $A(u) = \{-\Delta v : v \in \mathcal{V},\ u \in \mathcal{H},\ u \in \partial\Phi(v)\}$ on the domain

$Dom(A) = \{u \in \mathcal{H} : u \in \partial\Phi(v) \text{ for some } v \in \mathcal{V}\}$. To see that A is accretive on the Hilbert space $\mathcal{V}'$, we use (23) to compute for $\langle u_j, -\Delta v_j\rangle \in A,\ j = 1, 2,$

$$(u_1 - u_2, -\Delta(v_1 - v_2))_{\mathcal{V}'} = (u_1 - u_2, v_1 - v_2)_{\mathcal{H}} \geq 0$$

since $\partial\Phi$ is monotone. To verify that the operator is m-accretive, we need to solve the problem

$$u \in \mathcal{H},\ v \in \mathcal{V} : u - \Delta v = f,\ u \in \partial\Phi(v), \tag{35}$$

for each $f \in \mathcal{V}'$. The solution is characterized by

$$v \in \mathcal{V} : f(w - v) \leq \Phi(w) - \Phi(v) - \Delta v(w - v) \text{ for all } w \in \mathcal{V}, \tag{36}$$

with additionally $u \in \mathcal{H}$. This is resolved by standard results for monotone operators ([8, 34] or see [[51], *Theorem II.7.1*]), and then the affine bound

$$|\eta| \leq a|\xi| + b \text{ for all } \eta \in \beta(x; \xi),\ x \in \Omega,\ \xi \in \mathbb{R}, \tag{37}$$

together with the a-priori estimate $\|v\|_{\mathcal{V}} \leq C\|f\|_{\mathcal{V}'}$ from (36) imply that $u \in \mathcal{H}$.

Remark 3.5. *Here we have used the estimates from the elliptic operator $-\Delta$ to solve the resolvent equation. In the case of a single $\alpha = (\partial\varphi)^{-1}$, to show that $-\Delta \circ \alpha$ is a subgradient on $\mathcal{V}'$ one uses a coercivity estimate on the conjugate convex function φ^*, hence, $\alpha = \partial\varphi^*$ is necessarily onto.*

The preceding construction permits the application of Theorem 3.1 to obtain the the following result.

Theorem 3.3. *Assume $\Phi : \mathcal{H} \to \mathbb{R}_\infty$ is given by* (33) *as a normal convex integrand, and assume the subgradients $\beta(x; \xi) = \partial\varphi(x; \xi)$ satisfy* (37)*. Let $f \in W^{1,1}((0, T), \mathcal{V}')$ and $u_0 \in \partial\Phi(v_0)$ for some $v_0 \in \mathcal{V}$. Then there is a unique pair $u \in W^{1,\infty}((0, T), \mathcal{V}'),\ v \in L^\infty((0, T), \mathcal{V})$ which satisfies*

$$\tfrac{du}{dt} - \Delta v(t) = f(t) \text{ in } \mathcal{V}' \text{ for a.e. } t \in (0, T), \tag{38a}$$

$$u(t) \in \partial\Phi(v(t)) \text{ in } \mathcal{H},\ v(t) \in \mathcal{V} \text{ for all } t \in (0, T), \tag{38b}$$

$$u(\cdot, 0) = u_0(\cdot) \text{ on } \Omega. \tag{38c}$$

This is the weak solution of the initial-boundary-value problem (22).

Comparison principle. Here we establish a result which is the counterpart of the maximum principle quoted in Section 3.1 for the Stefan problem. For $j = 1, 2$ let

$$u_j - \Delta v_j = f_j \text{ in } L^1(\Omega),\ v_j \in W_0^{1,1}(\Omega),\ v_j(x) \in \alpha(x; u_j(x)) \text{ a.e. in } \Omega. \tag{39}$$

The approximate Heaviside function is given by $H_\varepsilon(v) = 0$ for $x \le 0$, $\frac{x}{\varepsilon}$ for $0 \le x \le \varepsilon$, and 1 for $\varepsilon \le x$; its limit is $H_0(v) = 0$ for $x \le 0$ and 1 for $0 < x$. The corresponding maximal monotone graph is the extension $H(\cdot)$ with $H(0) = [0, 1]$. We approximate (39) by replacing $\beta(x; \cdot) = \alpha(x; \cdot)^{-1}$ by its Yosida approximation, $\beta_\lambda(x; \cdot)$, $\lambda > 0$. Then $\alpha^\lambda(x; \xi) = \beta_\lambda^{-1}(x; \xi) = \alpha(x; \xi) + \lambda\xi$ is strictly increasing. The corresponding approximating problems are

$$u_j^\lambda - \Delta v_j^\lambda = f_j \text{ in } L^1(\Omega),\ v_j^\lambda \in W_0^{1,1}(\Omega),\ v_j^\lambda(x) \in \alpha^\lambda(x; u_j^\lambda(x)) \text{ a.e. in } \Omega. \tag{40}$$

We define $\sigma_\varepsilon = H_\varepsilon(v_1^\lambda - v_2^\lambda)$; since $\alpha^\lambda(x; \cdot)$ is strictly increasing, the limit as $\varepsilon \to 0$ satisfies

$$\sigma_\varepsilon \to H_0(v_1^\lambda - v_2^\lambda) \in H(u_1^\lambda - u_2^\lambda). \tag{41}$$

Subtract the equations (40) for $j = 1, 2$, multiply by σ_ε, integrate over Ω and compute

$$-\int_\Omega \Delta(v_1^\lambda - v_2^\lambda)\sigma_\varepsilon(x)\, dx = \int_\Omega |\nabla(v_1^\lambda - v_2^\lambda)|^2 H_\varepsilon'(v_1^\lambda - v_2^\lambda) dx \ge 0,$$

so dropping this term and taking limits as $\varepsilon \to 0$ yield

$$\int_\Omega (u_1^\lambda - u_2^\lambda) H_0(v_1^\lambda - v_2^\lambda)\, dx \le \int_\Omega (f_1 - f_2)_+\, dx,$$

where $w_+ = w\, H_0(w) = max\{w, 0\}$ denotes the positive part of w. Using (41), we obtain

$$\|(u_1^\lambda - u_2^\lambda)_+\|_{L^1(\Omega)} \le \|(f_1 - f_2)_+\|_{L^1(\Omega)}, \tag{42}$$

and letting $\lambda \to 0$ implies $u_j^\lambda \to u_j$ for $j = 1, 2$. This follows even in this x-parametrized case $\beta(x; \cdot)$ by the proof in [7]; see also the proof of Lemma 4.2. We obtain the following.

Lemma 3.1. *Assume u_1, u_2 are solutions of* (39)*. Then*

$$\|(u_1 - u_2)_+\|_{L^1(\Omega)} \le \|(f_1 - f_2)_+\|_{L^1(\Omega)}. \tag{43}$$

Consequently, if $f_1 \le f_2$, then $u_1 \le u_2$.

With a variation of this argument, we obtain an L^∞ bound on solutions of (39) for the methane hydrate example (20) when the constraint is subharmonic: we assume $-\Delta v^* \ge 0$. Set $u_2(x) = R$ and

$v_2^\lambda(x) = v_\lambda^*(x) = \alpha_{MH}^\lambda(x; R)$. Note that the boundary trace $v_2^\lambda|_{\partial\Omega}$ is positive. Define $f_2^\lambda = R - \Delta v_\lambda^* = u_2 - \Delta v_2^\lambda$. Let

$$u^\lambda - \Delta v^\lambda = f \le R \text{ in } L^1(\Omega),\ v^\lambda(x) = \alpha_{MH}^\lambda(x; u^\lambda(x)) \text{ in } W_0^{1,1}(\Omega).$$

Then $u^\lambda - u_2 - \Delta(v^\lambda - v_2^\lambda) = f - f_2^\lambda = \Delta v_\lambda^* \le 0$. Multiply this by $H_\varepsilon(v^\lambda - v_2^\lambda)$ and integrate. Since $v^\lambda - v_2^\lambda$ is negative on the boundary, $H_\varepsilon(v^\lambda - v_2^\lambda)$ vanishes there. The same calculations leading to (42) yield here $\|(u - u_2)_+\|_{L^1(\Omega)} \le 0$, so we obtain $u \le R$.

Corollary 3.1. *Assume the constraint satisfies $-\Delta v^* \ge 0$. Let u be the solution of*

$$u - \Delta v = f \text{ in } L^1(\Omega),\ v = \alpha_{MH}(\cdot; u) \text{ in } W_0^{1,1}(\Omega).$$

If $0 \le f(x) \le R$ a.e. in Ω, then $0 \le u(x) \le R$ a.e. in Ω.

The lower bound follows directly from Lemma 3.1 since $\alpha_{MH}(\cdot; 0) = 0$.

Now for two solutions $u_j(t), v_j(t)$ to the evolution problem (38) we are back to solving the implicit-in-time problems

$$\frac{u_j^n - u_j^{n-1}}{t^n - t^{n-1}} - \Delta v_j^n = f_j^n,\ v_j^n \in \alpha(x; u_j^n)\,, \tag{44}$$

where $j = 1, 2$, $u_j^0 = u_j(0)$, and the solutions of these stationary problems are in $L^1(\Omega)$. The estimate (43) carries over to the limit $u_j(t)$ of the time-discrete u_j^n and we have

$$\|(u_1(t) - u_2(t))_+\|_{L^1(\Omega)} \le \|(u_1(0) - u_2(0))_+\|_{L^1(\Omega)} + \int_0^t \|(f_1(s) - f_2(s))_+\|_{L^1(\Omega)} ds. \tag{45}$$

The reasoning here follows along the usual path, see, e.g., [[51], *p221*].

As before, for the methane hydrate example (20) with a subharmonic constraint, we can use the constant solution $u_2(t) = R \ge 0$ to bound a solution $u(t)$ of the initial-boundary-value problem (22). Using $v_2(t) = v^* = \alpha(x; R)$ and $f_2(t) = -\Delta v^*$, we obtain the following.

Corollary 3.2. *If $u(t), v(t)$ is a solution of (22) with $0 \le u(0) \le R$ and $0 \le f(t) \le -\Delta v^*$, then we have $0 \le u(t) \le R$.*

Remark 3.6. *The comparison principle lets us extend the graph β as before, so the results for Stefan problem apply. It also lets us formulate existence/uniqueness for the L^1 notion of solutions extending (27) for the case $\alpha = \alpha(x; \cdot)$.*

4. Numerical approximation

In this Section we discuss the numerical formulation to (4) with no sources. We are interested primarily in the situation when β and α are parameter-dependent graphs, so we generalize the results known for (2) and in particular for the Stefan problem with $\alpha = \alpha_{ST}$. We review the latter in Section 4.1.

For discretization of a general monotone evolution equation (2) two interrelated difficulties arise. The first is the (in)sufficient regularity of solutions which prevents establishing an optimal convergence order. The second difficulty is with solving the nonlinear algebraic problem resulting from the discretization. For implicit schemes, Newton-type solvers have difficulties near singularities, and are not even defined for multivalued operators. On the other hand, relaxation solvers apply easily but require the number of iterations to be proportional to the number of degrees of freedom.

In Section 4.2 we propose a scheme for (4) which does not require regularization, is fully implicit, and can be applied when neither α nor β are functions as well as when they are parametrized by x as in (4). We propose a solver from a class of semi-smooth Newton methods [54]; these were only recently proposed for applications similar to the ones considered here [29, 23, 25], and they converge in just a few iterations. We discuss the main ideas behind the semismooth solver in Section 4.3 and show how to use it for graphs from Section 3.1.1, and in particular, for the Stefan problem. Numerical results are presented in Section 5.

4.1. **Numerical schemes for** (2)**.**

The literature on numerical discretization of (2) and in particular for the Stefan problem is extensive, and we do not attempt a detailed review. Rather, we recall the known solver and convergence issues. We first discuss semidiscrete approximations in time, then fully discrete schemes. For simplicity, we assume here uniform time-stepping with time step τ, thus $t_n = n\tau$.

4.1.1. *Semidiscrete discretization for* (2).

A convenient way to define and analyze discrete schemes for (25) is via semigroup theory. If A is given as in (26), it is known that $-A$ is the generator of a nonlinear semigroup of contractions $\{S_A(t) : t \geq 0\}$ on $L^1(\Omega)$, and the solution $u(t)$ of the initial-value problem is obtained as the limit of the implicit finite-difference scheme (cf. (44))

$$\frac{u^{n+1} - u^n}{\tau} - \Delta\alpha(u^{n+1}) = 0. \tag{46}$$

The semigroup is given by $S_A(t)u_0 = \lim_{n\to\infty}(I + \frac{t}{n}A)^{-n}u_0$. The numerical analysis of optimal convergence rates for the fully discrete problem based on the implicit scheme (46) was given in [44, 45]. This set of results does not require regularization.

Semi-implicit schemes analyzed in [3, 56] take advantage of the linear factor $-\Delta$ of the operator A when $\alpha(\cdot)$ is a Lipschitz function. In particular, the approximation of $-\Delta$ by its generated semigroup $\{S_{-\Delta}(t)\}$, gives the scheme

$$\frac{u^{n+1}-u^n}{\tau}+\frac{1}{\tau}(I-S_{-\Delta}(\tau))\alpha(u^n)=0, \tag{47}$$

which can be implemented using Euler's, Crank-Nicolson etc.; see [[3], *eq.(9b)*] or [[56], *eq.(14)*] for early solution to the Stefan problem. Another scheme takes the form

$$\frac{u^{n+1}-u^n}{\tau}+\frac{1}{\tau}(I-(I-\tau\Delta)^{-1})\alpha(u^n)=0, \tag{48}$$

in which Yosida's approximation has been used for the linear $-\Delta$. This scheme is also explicit in the nonlinear term but relies on an approximate solver for the linear elliptic resolvent $(I-\tau\Delta)^{-1}$). See [[3], *(eq.19)*] or [[56], *(eq.26)*]. The semi-implicit schemes (47)-(48) can be analyzed using Chernoff formulae for the nonlinear semigroup. When combined with spatial discretization, they require that stability restrictions on the time step must be met. Below we only consider fully implicit schemes for (4).

4.1.2. *Fully discrete implicit schemes for* (2). The schemes combining (46) with finite element discretizations in space have been defined for various degenerate and singular parabolic problems; see overview of applications in [38, 19]. Consider the usual finite element space $\mathcal{V}_h\subset\mathcal{V}$ spanned by piecewise linears over a triangulation of Ω [12] and an associated interpolant I_h with range in $\mathcal{V}_h$. The scheme involves the solutions in $v_h^n\in\mathcal{V}_h$ at each discrete time step $t_n, n>0$ of

$$(u_h^n,\psi)+\tau(\nabla v_h^n,\nabla\psi) \quad = \quad (u^{n-1},\psi),\ \ \forall\psi\in\mathcal{V}_h\,, \tag{49a}$$

$$u_h^n\in\beta_h(v_h^n)\,, \tag{49b}$$

$$(u_h^0,\psi) \quad := \quad (u_0,\psi)\,, \tag{49c}$$

where the crucial definition of u_h^n,β_h is made clear below.

We recall briefly the numerical analyses of (49) in which β is multi-valued such as in the Stefan problem. We are mostly interested in the convergence results in $L^2(Q)$ which are the easiest to verify. Here and below we denote $Q=\Omega\times(0,T)$. A quasi-norm convergence quantity q to be defined later is considered, e.g., in [19]. Convergence results in other norms such as $L^\infty((0,T),\mathcal{V}')$ are also known from the literature but will not be used here.

The numerical solution of permafrost thawing described in [58] inspired theoretical analyses in [27] and a discussion of the Newton method in [28]. In [58] β is actually a continuous globally Lipschitz

function $u = \beta(v) = v + LH_p(v)$ where $H_p(v) \sim (\frac{a}{a-v})^4$, and a is a parameter determined experimentally. However, the results in [27] and [28] are derived for the singular Stefan problem where $u = \beta(v) = v + LH(v)$. For the Stefan problem and $\beta^{-1} = \alpha_{ST}$, an extensive collection of results in [21, 56, 27, 28, 37, 38, 35, 36, 45] have been developed, and they cover the convergence of the algorithms, the use of numerical integration, solver issues, and adaptive gridding.

The convergence analysis in most of the papers assumes α is Lipschitz and takes advantage of regularizations β_ϵ of β, see [27, 37, 38], and (under possibly additional assumptions) shows that the error in v is $O(h)$ if only τ and the regularization parameter are selected appropriately. Part of the analysis is devoted to accounting for inconsistency between the solutions (u_ϵ, v_ϵ) of the regularized problem and (u, v) solving (2). As $\epsilon \to 0$, the inconsistency gets smaller; however, the constants in approximations blow up, and thus one has to adjust ϵ to h. Since $\beta_h = \beta_\epsilon$ is a function, the choice in (49b) is unambiguous by defining u_h^n as the finite element interpolant $I_h\beta_\epsilon(v_h^n)$, i.e., $u_j = u_h(x_j) = \beta_\epsilon(v_h(x_j))$ at all nodal points x_j of the finite element grid; see, e.g., [[38], *p792*]. The regularizations are also used in implementation; most use a nonlinear relaxation iterative solver analyzed in [21, 36].

Analysis without regularization is discussed in [45] and some theoretical results proven in [27] are extendable to the non-regularized version; see also the stationary problem discussed in [21] for which some (sub)optimal results were derived. Here the selection out of $\beta(v_h(x_j))$ is, in general, not unique, unless one makes precise how (49) is solved. A duality argument employed in [[45], *Lemma 2.4*] shows uniqueness of the pair $\langle u_h^n, v_h^n\rangle$ with u_h^n identified as the (unique) $\mathcal{H}$-projection onto $\mathcal{V}_h$ of an element out of $\beta(v_h(x_j))$. Thereby β_h has a unique meaning.

In summary, theoretical and practical results in [37, 27] suggest that the best convergence orders are close to $O(h)$ and $O(h^{\frac{1}{2}})$ in $L^2(Q)$ for v and u, respectively. These were demonstrated for Lipschitz α, smooth initial data, and for regularized schemes, with $\tau = O(h^r)$, and r chosen to be $\frac{2}{3}$ if additional properties can be assumed, or larger without it. These rates were confirmed to hold for the Stefan problem in [38].

4.2. **Fully discrete scheme for** (4)**.** For graphs such as (30) or parameter-dependent families (20) no results are available in the literature. However, a scheme can be readily defined to extend (49). The first equation (49a) is unchanged; we rewrite it in a matrix-vector form whereby $v_h^n \approx \mathbf{v}^n \in \mathbb{R}^M$ are identified by its degrees of freedom $(v_1, \ldots v_M)$. Let $\mathbf{M}$ and $\mathbf{K}$ be the usual mass and stiffness matrices defined by $(u_h, w_h) = \mathbf{w}^T\mathbf{M}\mathbf{u}$ and $(\nabla u_h, \nabla w_h) = \mathbf{w}^T\mathbf{K}\mathbf{u}$ for any $u_h, w_h \in V_h$, and thus (49a) can be written as $\mathbf{M}\mathbf{u}^n + \tau\mathbf{K}\mathbf{v}^n = \mathbf{M}\mathbf{u}^{n-1}$. Instead of the $L^2(\Omega)$ inner products (w, ψ) in (49a), one can use

their approximations $(w, \psi)_h$ via numerical integration, i.e., mass lumping (see [38]). In that case, in 1D on a uniform grid, $\mathbf{M}$ is replaced by $h\mathbf{I}$. Its special structure is exploited below.

In summary, our discrete problem is

$$\mathbf{u}^n + \tau \mathbf{A}_h \mathbf{v}^n = \mathbf{u}^{n-1} \tag{50a}$$

where $\mathbf{A}_h$ is $\mathbf{M}^{-1}\mathbf{K}$. Note that $\mathbf{A}_h$ is symmetric and positive definite. It remains to identify β_h as in (49b). It is natural to use the pointwise selection

$$\langle v_j^n, u_j^n \rangle \in \beta(x_j; \cdot) := \beta_j(\cdot). \tag{50b}$$

When complemented by initial selection such as (49c), the discrete scheme is complete.

Now we show that the scheme (50) is uniquely solvable, at least for all the examples from Section 3.1.1. This follows from an argument similar to that used to establish the range condition in (34). For a closed convex set K, the convex lower semicontinuous indicator function $I_K(x)$ is 0 for $x \in K$ and $+\infty$ otherwise.

Lemma 4.1. *For every $n > 0$ there is a unique solution in $\mathbf{v}^n \in \mathbb{R}^M$ of (50) for $\beta = \beta_{MH}$; it is the unique minimizer of the appropriate functional $\Psi(\mathbf{v})$ for which (50) is the Euler-Lagrange condition.*

Proof. Consider the problem solved at every time step for $\mathbf{u} = \mathbf{u}^n$ and $\mathbf{v} = \mathbf{v}^n$

$$\mathbf{u} + \tau \mathbf{A}_h \mathbf{v} = \mathbf{f},\ u_j \in \beta_j(v_j),\ j = 1, 2, ..., M. \tag{51}$$

For $\beta = \beta_{MH}(x; \cdot)$ in (20) we must define $\Psi(\mathbf{v}) = \Psi_{MH}(\mathbf{v})$. Consider pointwise-defined convex functions $\varphi_j(\lambda) = \frac{1}{2}\lambda^2 + I_{(-\infty, v^*(x_j)]}(\lambda)$ and $\Phi(\mathbf{v}) := \sum_j \varphi_j(v_j)$. Now $\beta(x_j, \cdot) = \partial\Phi$. Since $\mathbf{A}_h\mathbf{v}$ defined on all of $\mathbb{R}^M$ is single-valued, thus maximal, we also have, by [[51], *Prop. II.7.7*] that the subgradient $\partial\Psi(\mathbf{v})$ of $\Psi(\mathbf{v}) = \frac{1}{2}\tau\mathbf{v}\mathbf{A}_h\mathbf{v}^T + \Phi(\mathbf{v})$ is equal to $\tau A_h\mathbf{v} + \partial\Phi(\mathbf{v})$, and this completes the proof. □

From the proof of Lemma 4.1, it is clear how to show solvability also for $\beta = \beta_E$ and β_W: this follows by defining appropriate convex functions $\varphi_E = I_{(-\infty,1)}$ and $\varphi_W(x) = x + I_{[0,\infty)}$, respectively. For β_{ST}, the construction used to establish Lemma 4.1 is that of [[21], *1.8,2.2,3.4*] with $\varphi_{ST}(\lambda) = \frac{1}{2}\lambda^2 + \lambda_+$.

We summarize the results in the Corollary.

Corollary 4.1. *The scheme (50) is uniquely solvable for each of $\beta = \beta_{MH}(x, \ )$, β_{ST}, β_E, β_W.*

Remark 4.1. *Convergence of the solutions to (50) has been rigorously established in the literature only for the Stefan problem. It is easy to see that these can be extended to β_{MH} when $v^* \equiv const$ as long as*

an appropriate comparison principle lets us extend that graph to one that is affine bounded so that the theory in [38] *applies. The general case of nonconstant* v^* *requires more work and will be considered elsewhere.*

We now prove the comparison principle for the simplified case of $d = 1$ with mass lumping and uniform grid. The proof is different from that for Lemma 3.1 because it does not require approximation H_ε to the Heavisde function H.

Lemma 4.2. *Consider the case of* (50) *for which* $\mathbf{A}_h$ *is the usual tridiagonal discrete Laplacian scaled by* $\frac{1}{h^2}$. *Let solutions* $\mathbf{u}^{(1)}, \mathbf{u}^{(2)}$ *with the corresponding* $\mathbf{v}^{(1)}, \mathbf{v}^{(2)}$ *satisfy* (51) *for* $\mathbf{f} = \mathbf{f}^{(1)}, f^{(2)}$, *respectively. Let also* $v_j^{(1)} - v_j^{(2)} = 0$ *for boundary indices* j. *Then the counterpart of* (43) *holds, namely,*

$$\sum_{j=1}^{M} (\mathbf{u}^{(1)} - \mathbf{u}^{(2)})_+ \le \sum_{j=1}^{M} (\mathbf{f}^{(1)} - \mathbf{f}^{(2)})_+ \,. \tag{52}$$

Proof. In the case considered we solve (51) for vectors $\mathbf{u} = (u_1, \dots u_M), \mathbf{v} = (v_1, \dots v_M)$ with v_0, v_{M+1} set from boundary conditions. Denote $D_{j+1}\mathbf{v} = \tau \dfrac{v_{j+1} - v_j}{h^2}$. From (51) we have, for $j = 1, \dots M$,

$$u_j + (D_j \mathbf{v} - D_{j+1}\mathbf{v}) = f_j,\ u_j \in \beta_j(v_j),$$

Subtracting this identity written for $\mathbf{u}^{(m)}, \mathbf{v}^{(m)}$ for $m = 1, 2$, setting $\mathbf{w} = \mathbf{v}^{(1)} - \mathbf{v}^{(2)}$, multiplying both sides by $H(w_j)$, and summing we obtain

$$\sum_j H(w_j)(u_j^{(1)} - u_j^{(2)}) + \sum_j H(w_j)(D_j \mathbf{w} - D_{j+1}\mathbf{w}) = \sum_j H(w_j)(f_j^{(1)} - f_j^{(2)}). \tag{53}$$

Since $H(w_j) \in [0, 1]$, thus $H(w_j)(f_j^{(1)} - f_j^{(2)}) \le (f_j^{(1)} - f_j^{(2)})_+$, and so the right side of (53) is bounded by that of (52).

Next, by summation by parts we calculate

$$\sum_{j=1}^{M} H(w_j)(D_j \mathbf{w} - D_{j+1}\mathbf{w})$$
$$= \frac{\tau}{h^2} \left(H(w_1)(w_1 - w_0) + H(w_M)(w_M - w_{M+1}) + \sum_{j=2}^{M} (H(w_j) - H(w_{j-1}))(w_j - w_{j-1}) \right).$$

Since H is monotone, every component of the sum in the last term is nonnegative, and so are the terms $H(w_j)w_j, j = 1, M$. Now, if $\mathbf{v}^{(m)}$ both satisfy the same boundary conditions, and in particular if $v_j^{(m)} = 0$ for $j = 0, M + 1$, then the entire sum is nonnegative, so the second part of the left side of (53) is nonnegative.

It remains to deal with the first term in (53). If β_j is single valued, pointwise we have $H(w_j)(u_j^{(1)} - u_j^{(2)}) = H(v_j^{(1)} - v_j^{(2)})(u_j^{(1)} - u_j^{(2)}) = (u_j^{(1)} - u_j^{(2)})_+$. In the multivalued case, we proceed by using its single-valued Yosida regularization β_j^λ defining the corresponding families $\mathbf{u}_\lambda, \mathbf{v}_\lambda, \mathbf{w}_\lambda$ and proving the result for these. Passing to the limit with $\lambda \to 0$ as in [7], see also [[51], *Thm II.9.2*], we obtain the desired result. □

Remark 4.2. *Note that our proof of Lemmas 4.1,4.2 did not require that either α or β be single-valued, thus they apply to all Examples from Section 3.1.1.*

As for solving the algebraic problem (50), an (iterative) relaxation solver is proven to converge linearly in [21]. However, as shown, e.g., in [36], it requires the number of iterations proportional to the number of degrees of freedom. In contrast, semismooth Newton methods converge superlinearly and generally require only a few iterations. This is discussed in the sequel.

4.3. **Semismooth solver.** To solve (50) with semismooth Newton methods, the main idea is to use not just one but a double set of degrees of freedom corresponding to the two unknowns $\mathbf{u}, \mathbf{v}$ simultaneously, and to replace (50b) by (5). If the graph β has piecewise smooth pieces, one can show that ϕ is semismooth. Also, the resulting Jacobian is never singular which we can show based on monotonicity of β, and one concludes that the semismooth Newton algorithm converges superlinearly.

For the methane hydrate application that originally motivated this paper the graph β_{MH} can be described in a natural way using a complementarity constraint (CC). For finite dimensional problems with CCs it is very efficient to use a solver from the class of semismooth Newton methods [54]. We extend this observation further and see that CC-based semismooth Newton solver can be used for any application in which β can be expressed as a CC. In particular, the semi-smooth solver applies readily to the Stefan problem (29), without regularization, and to the graph given by (30). We elaborate below on the details of a CC-based solver.

4.3.1. *Formulation of $u \in \beta(u)$ as an NCC.* From now on we fix n and suppress it as superscript.

It is useful [29, 54, 23] to rewrite

$$\begin{cases} \lambda \geq 0, & \mu = 0, \\ \lambda = 0, & \mu \geq 0, \\ \mu\lambda & = 0 \end{cases} \tag{54}$$

as $\phi(\lambda, \mu) = \min(\lambda, \mu) = 0$. This is advantageous when setting up the numerical solution of systems with CC such as (54).

More generally, let $\langle u, v\rangle \in \beta$ be represented as a NCC in the form $\min(F(u,v), G(u,v)) = 0$, where F, G are some smooth functions. Thus (50) is solved together as

$$\mathbf{u} + \tau \mathbf{A}_h \mathbf{v} = \mathbf{b}, \tag{55a}$$

$$\min(F_j(u_j, v_j), G_j(u_j, v_j)) = 0, \ \forall j, \tag{55b}$$

with $\mathbf{b}$ given from the previous time step.

We apply semismooth Newton methods to solve (55). The Jacobian $\mathbf{J} = \begin{bmatrix} \mathbf{J}_{11} & \mathbf{J}_{12} \\ \mathbf{J}_{21} & \mathbf{J}_{22} \end{bmatrix}$ of (55) has a block structure in which $\mathbf{J}_{21}, \mathbf{J}_{22}$ are diagonal. In addition, $\mathbf{J}_{11} = \mathbf{I}, \mathbf{J}_{12} = \tau \mathbf{A}_h$ are constant, hence smooth in u, v but $\mathbf{J}_{21}, \mathbf{J}_{22}$ are only semismooth due to non-differentiability of the function $\min(r, s)$ across the line $r = s$.

Let $J^- := \{j : F(u_j, v_j) - G(u_j, v_j) < 0\}$, and J^+, J^0 are defined analogously. We see $(\mathbf{J}_{21}(\mathbf{u}, \mathbf{v}))_{jj} = \frac{\partial}{\partial u_j} \min(F(u_j, v_j), G(u_j, v_j))$ is equal to $\frac{\partial F}{\partial u_j}$ when $j \in J^-$, and to $\frac{\partial G}{\partial u_j}$ on J^+. The set J^0 on which the $\min(\cdot, \cdot)$ function is not differentiable can be lumped in implementation with J^-, so that one-sided derivative can be defined. One calculates $(\mathbf{J}_{22}(\mathbf{u}, \mathbf{v}))_{jj}$ analogously.

Since F, G are generally smooth, ϕ in (55b) is piecewise smooth, hence, semismooth [[54], *Proposition 2.23, p.34*]. For semismooth J it was shown in [[54], *Prop. 2.12, p. 29*] that Newton iteration converges superlinearly, if only $\mathbf{J}^{-1}(\mathbf{u}^{(k)}, \mathbf{v}^{(k)})$ can be shown bounded for any iterate $(\mathbf{u}^{(k)}, \mathbf{v}^{(k)})$ (condition (i) in [[54], *Prop. 2.12*]). In our examples the Jacobian is piecewise constant, and we just have to check that it is nonsingular; this is done separately for each application.

4.3.2. *Singular graph.* We can write (30) in the equivalent forms

$$u \in \beta_E(v) \Leftrightarrow \phi_E(u, v) := \min(u, 1 - v) = 0. \tag{56}$$

Corollary 4.2. *The semismooth Newton algorithm converges superlinearly for the problem* (30)*, for any initial guess.*

Proof. Since the functions $F(u, v) = u; G(u, v) = 1 - v$ are smooth, we see that the Jacobian $\mathbf{J}$ is constant on each J^-, J^+, J^0. We now show it is never singular.

Notice that $\mathbf{J}_{21}, \mathbf{J}_{22}$ are diagonal matrices with entries $(J_{21})_{jj} = \chi_{J^{-,0}}(j)$ and $(\mathbf{J}_{22})_{jj} = -\chi_{J^+}(j)$. Here χ_S is the characteristic function of set S equal to 1 for indices in S and equal 0 otherwise. To show $\mathbf{J}$ is nonsingular, we check if there are nontrivial solutions to $\mathbf{J}[\mathbf{u}, \mathbf{v}]^T = [0, 0]^T$ for $\mathbf{u}, \mathbf{v}$. From the form of $\mathbf{J}_{21}$ and $\mathbf{J}_{22}$ we see that the entries $\mathbf{u}^{-1,0}$ of $\mathbf{u}$ must vanish on $J^{-,0}$ and the entries $\mathbf{v}^+$ of $\mathbf{v}$ vanish on $J^{+,0}$. Next we seek the entries $\mathbf{u}_+$ and $\mathbf{v}^{-,0}$ that satisfy $(M\mathbf{u}_+)_j = 0$ on J^+ and $(K\mathbf{v}^{-,0})_j$

on $J^{-,0}$. Since M, K are positive definite on $J = \{1, \dots M\}$, they are positive definite on every subset of J. Thus the only solution is trivial with $\mathbf{u}_+ = \mathbf{0}$ and $\mathbf{v}_- = \mathbf{0}$, thus $\mathbf{J}$ is nonsingular.

We note in passing the following about any iterate $\mathbf{u}^{(k-1)}, \mathbf{v}^{(k-1)}$. Assume the set J^+ is nonempty. Then for $j \in J^+$ we have an equation defining the new iterate $(\mathbf{J}_{22})_{jj}(v_j^{(k)} - v_j^{(k-1)}) = (-1)(v_j^{(k)} - v_j^{(k-1)}) = -(1 - v_j^{(k-1)}) = -\phi(u_j^{(k-1)}, v_j^{(k-1)})$ thus we obtain $v_j^{(k)} = 1$, and these values can be used to eliminate v_j from the rows involving $\mathbf{J}_{11}, J_{12}$. Similarly, for any $j \in J^{-,0}$ we obtain $u_j^{(k)} = 0$. □

4.3.3. *The methane hydrate problem.* Equivalent forms for the methane hydrate problem (20) are

$$u \in \beta_{MH}(v) \Leftrightarrow \phi_{MH}(u, v) \equiv \min(u - v, v^*(x) - v) = 0, \tag{57}$$

whereas the original constraint in (v, S) can be written as

$$\min(v^*(x) - v, 1 - S) = 0. \tag{58}$$

Corollary 4.3. *The semismooth Newton algorithm converges superlinearly for the problem* (20) *and is equivalent to switching of variables.*

Proof. The proof of nonsingularity of $\mathbf{J}$ is similar to that for 4.2 is immediate, where the sets J^-, J^0, J^+ are now defined based on $\min(v^*(x_j) - v_j, 1 - S_j)$. In particular, $j \in J^+$ if $v^*(x_j) - v_j < 1 - S_j$.

As for variable switching, we consider an iterate $\mathbf{v}^{(k-1)}, \mathbf{S}^{(k-1)}$. The entries of $\mathbf{S}^{(k)}$ for $j \in J^{-,0}$ are set to $S_j^k = 1$ and thus one can say that the "independent variables" in these rows are v_j. Analogously, S_j are independent variables in rows corresponding to $j \in J^+$. The process thus is equivalent in implementation to that known as "variable switching" described in [22, 13]. □

In practice, merely a few iterations are needed for convergence, as will be shown in Section 5.

4.3.4. *The Stefan problem using MCP.* For the Stefan problem the entire graph (29) cannot be represented as a single NCC, but its pieces can. The bottom part of $\beta_{ST} = \alpha_{ST}^{-1}$ in (29) can be written as $\min(u - v, -v) = 0$, and is similar to a translate of the graph from (57) with $v^* \equiv 0$. The top part, written as $\min(1 + v - u, v) = \min(1 - (u - v), v) = 0$ is a "reflection" of the other part.

To define the entire graph β_{ST}, we use box (bilateral) constraints. Upon setting $w = u - v$, we see that $\langle v, w \rangle \in H$, and H is given as (6). Next we use the framework of MCP (mixed complementarity problems) as suggested in [[54], *(1.20-1.21),p8*], with which (6) is expressed equivalently as

$$y - m_{ST}(y + x) := y - \max(0, \min(y + x, 1)) = 0. \tag{59}$$

(A related approach is given in [[24], *p203*].) Thus

$$u \in \beta_{ST}(v) \Leftrightarrow \phi_{ST}(u,v) := u - v - m_{ST}(u) = 0\,. \tag{60}$$

This translates easily to $v = u - m_{ST}(u) = \alpha_{ST}(u)$, which is the same as (29). Furthermore, ϕ_{ST} is semismooth, just as ϕ_E, ϕ_{MH} are, and the corresponding Jacobian is never singular analogously to the case in (57).

Corollary 4.4. *The semismooth Newton algorithm converges superlinearly for the problem* (29)*.*

Because of the structure of ϕ_{ST}, there are three nontrivial sets of indices for the Stefan problem, and the number of iterations, especially for larger time steps, slightly exceeds that for methane hydrate problem.

5. Numerical results

Now we provide results of numerical experiments for (4) in $d = 1$ using the discrete scheme (50) and semismooth Newton solver. We are interested in convergence of the algorithms as well as in the behavior of the solver. The examples extend the results known for (2), either because α and β are not functions, or because α is parameter-dependent. We demonstrate that the discrete algorithm (50) works at least as well as the methods originally proposed for the Stefan problem. While we do not attempt a direct comparison of the solvers or of convergence rate, we show that $L^2(Q)$ errors in u are approximately of order $O(h^{\frac{1}{2}})$ while those in v are $O(h)$.

For all examples we run experiments for $\Omega = (0,1)$, $T = 0.13$ with various $M = 1/h$ and τ which varies as $O(h)$ or $O(h^2)$. We use close to machine precision tolerance in the Newton solver. We report on the convergence of the numerical solutions using $L^p(Q), p = 1, 2$ norms of the error in u and v, as well as on the quasi-norm as suggested in [19] and as seen in the proof [[45], *Thm 2.1*]

$$e_{u,p} := \left(\sum_n \tau \parallel u - u_h^n \parallel^p_{L^p(\Omega)} \right)^{1/p}, \tag{61}$$

$$e_{v,p} := \left(\sum_n \tau \parallel v - v_h^n \parallel^p_{L^p(\Omega)} \right)^{1/p}, \tag{62}$$

$$e_q := \sum_n \tau \int_\Omega |u - u_h^n||v - v_h^n| dx\,. \tag{63}$$

By comparing the solutions computed for different grids we are able to determine the rate of convergence, e.g., $r_{u,p}$ in $e_{u,p} = O(h^{r_{u,p}})$. We also define errors $e_{S,p}$ in saturations.

If the true solution u is not known, as in some examples below, we approximate $e_{u,p}$ by using $u \approx u_{h_{min}}$ computed on a very fine grid with h_{min} (and corresponding τ_{min}) approximately smallest h used in the tests. The same is done for v. In cases when the true solution is known, we have verified (but do not show it here) that this method is quite accurate but slightly (less than 10%) overpredicts $r_{u,p}$ as h gets closer to h_{min}.

In Tables below we report on the errors $e_{u,2}, e_{v,2}, e_q$ whose rate for rough solutions, as predicted by the theory reviewed in Section 4.1, should be at best $1/2, 1, 1$, respectively. We find that some of our rates appear higher because some of the solutions are smoother. In addition, we report on $e_{u,1}, e_{v,1}$ which are easy to compute but are not covered by the theory. These appear to be near 1 in all cases.

In addition, we show that the average number of Newton iterations N_{it} for all the problems is mesh-independent and in fact very small (in none of the cases shown did the number of iterations at any time step exceed 13). Note that we are not using any line-search or other globalization methods for Newton iterations. In spite of this, the problems require very few iterations to converge, which suggests robustness of the semismooth Newton implementation. Since our time-steps are chosen with convergence in mind and are rather small, our examples are possibly not challenging enough for the Newton algorithm. A more extensive study is needed to fully support our current conjectures on the superiority of semismooth-based solver over other solvers.

5.1. **One-phase Stefan problem.** We recall here an example with an analytical solution $v(x,t)$ in $d = 1$ from [[11], *17.3,p287*] derived for the one-phase Stefan problem. Consider a parameter $\lambda > 0$ which defines the boundary condition $v(0,t) = \lambda, t > 0$ at the left end of the domain, and assume the initial condition $u(x,0) = v(x,0) = 0$.

There is only one "phase" in the problem, and v is nonnegative everywhere, and positive only ahead of the free boundary $x = s(t)$, with $v(s(t),t) = 0$. Therefore $u(x,t) = v(x,t) + 1$ for $x < s(t)$ ahead of the free boundary, and there is a jump down to the value $u(x,t) = v(x,t)$ for $x > s(t)$ behind the free boundary.

The evolution is considered for t not exceeding the time t^s when the front of the free boundary reaches $x = 1$, so that the right boundary condition $v(1,t) = 0, t \le t^s$ holds. In fact, v satisfies

$$v_t - v_{xx} = 0,\ 0 < x < s(t), 0 < t < t^s \tag{64a}$$

$$v(x,0) = 0,\ 0 \le x,\ v(0,t) = \lambda \tag{64b}$$

TABLE 1. Convergence and iteration count for (64)

$1/h$	$1/\tau$	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
32	320	2	2.43e-02		2.27e-03		5.42e-03		6.32e-04		6.25e-03	
64	640	2	1.69e-02	0.523	1.14e-03	0.983	3.45e-03	0.651	3.30e-04	0.936	3.81e-03	0.714
128	1280	2	1.17e-02	0.535	5.70e-04	1.011	2.10e-03	0.713	1.67e-04	0.979	2.25e-03	0.758
256	2560	2	7.91e-03	0.566	2.76e-04	1.044	1.24e-03	0.760	8.27e-05	1.020	1.31e-03	0.784
512	5120	2	5.22e-03	0.600	1.30e-04	1.082	7.06e-04	0.818	3.90e-05	1.083	7.33e-04	0.837
16	1600	2	3.22e-02		3.40e-03		5.20e-03		4.83e-04		8.51e-03	
32	3200	2	2.23e-02	0.533	1.67e-03	1.024	1.92e-03	1.438	1.73e-04	1.482	4.24e-03	1.007
64	6400	2	1.55e-02	0.525	8.29e-04	1.015	8.33e-04	1.204	6.99e-05	1.308	2.17e-03	0.963
128	12800	2	1.06e-02	0.548	4.03e-04	1.041	4.23e-04	0.978	2.98e-05	1.227	1.10e-03	0.972
256	25600	2	6.98e-03	0.603	1.88e-04	1.093	2.27e-04	0.897	1.27e-05	1.225	5.55e-04	0.998
16	256	2	3.19e-02		3.72e-03		5.65e-03		7.59e-04		8.29e-03	
32	1024	2	2.13e-02	0.581	1.69e-03	1.136	2.32e-03	1.282	2.47e-04	1.617	4.13e-03	1.003
64	4096	2	1.40e-02	0.609	7.72e-04	1.133	9.62e-04	1.272	8.24e-05	1.588	2.07e-03	1.000

and this case is a special case of (2) with (29). To find the free boundary, solve for $c = c(\lambda)$ the identity

$$\lambda = c\exp(\frac{c^2}{4})\int_0^{\frac{c}{2}} \exp(-r^2)dr. \tag{65}$$

It is not hard to see that the right hand side of this identity is monotone in c thus the solution can always be found. We find $c(\lambda)$ numerically, e.g., for $\lambda = 2$ we obtain $c(\lambda) = 1.6012$. Then the free boundary is $s(t) = c\sqrt{t}$, and we have

$$v(x,t) = \lambda - c\exp(\frac{c^2}{4})\int_0^{\frac{x}{2\sqrt{t}}} \exp(-r^2)dr,\ x < s(t). \tag{66}$$

For this problem we show the results of our simulations in Table 1. The computed L^2 rates agree with the theory, and they depend on the scaling between h and τ, while L^1 rates are generally higher.

5.2. **Singular graph with an analytical solution.** Here we recall the example (30) from [50] in which neither the maximal monotone graph α nor its inverse is continuous, but both are affine-bounded. Here we can extend (30) to $\alpha(0) = [0,1]$, $\alpha(x) = \{1\}$ for $0 < x \le 1$, and $\alpha(x) = x$ for $x \notin [0,1]$.

Define a pair of functions, u, v as follows. Set $u(x,t) = 1$ for $0 \le t < 1/8$, $\sqrt{2t} < x < 1 - \sqrt{2t}$, and $u(x,t) = 0$ otherwise. Let $v(t) \in H_0^1(0,1)$ be given by $v(x,t) = \min\{x/\sqrt{2t},\ 1,\ (1-x)/\sqrt{2t}\}$ for $0 < x < 1$, $0 < t < 1/8$, and $v(x,t) = 0$ otherwise. These functions are the solution of the initial-boundary-value problem

$$u_t - v_{xx} = 0,\ v \in \alpha_E(u), \tag{67a}$$

$$v(\cdot,t) \in H_0^1(0,1) \text{ for } t > 0,\ u(x,0) = 1. \tag{67b}$$

That is they are solutions according to both (27) and (28), but *neither* is continuous on $(0,1)\times(0,\infty)$.

Note that this example is not covered by the theory of convergence from [45] since α is not a function. Still, we observe in Table 2 that the convergence rates are similar as for (64) in u, but with no superconvergence for v.

TABLE 2. Convergence and iteration count for (67)

$1/h$	$1/\tau$	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
32	320	2	3.04e-02		2.92e-03		5.88e-03		8.79e-04		4.78e-03	
64	640	2	2.14e-02	0.502	1.49e-03	0.973	3.51e-03	0.743	4.82e-04	0.867	2.57e-03	0.893
128	1280	2	1.50e-02	0.515	7.42e-04	1.006	2.05e-03	0.771	2.42e-04	0.993	1.34e-03	0.934
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
16	1600	2	4.33e-02		5.84e-03		9.44e-03		1.88e-03		1.16e-02	
32	3200	2	3.06e-02	0.498	2.98e-03	0.969	4.77e-03	0.986	9.40e-04	1.001	5.93e-03	0.971
64	6400	2	2.15e-02	0.513	1.49e-03	0.997	2.39e-03	0.993	4.71e-04	0.999	2.99e-03	0.987
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
16	256	2	4.15e-02		5.43e-03		1.01e-02		1.90e-03		9.44e-03	
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

5.3. **Singular graph with a constant solution.** In this example we use $\alpha - \alpha_W$ given by (31) extended as in previous section by $\alpha(x) = x$ for $x \notin [0,1]$. It is straightforward to check that the constant solution $u \equiv 1/2, v \equiv 0$ satisfies

$$u_t - v_{xx} = 0,\ v \in \alpha_W(u), \tag{68a}$$

$$v(\cdot,t) \in H_0^1(0,1) \text{ for } t > 0,\ u(x,0) = 1/2. \tag{68b}$$

Notice that $\beta_W = \alpha_W^{-1} = \alpha_E$ represents the upper part of Heaviside graph; this example was used in [[28], *p863*] to demonstrate the need for line searching in a regular Newton algorithm, without which the authors suggest the algorithm would not converge if given an positive initial guess fror v.

With semismooth Newton algorithm and $\phi_W(u,v) = \min(1-u, v)$ we find that the algorithm converges after 2 iterations to the true solution, and line search is not needed.

Since the numerical solution trivially matches the analytical (constant) solution, we do not report on the errors.

5.4. **Methane hydrates problem.** If $v^* = const$, then the graph α_{MH} is a translate of (a one-phase portion of) α_{ST} and thus we expect the results to be not worse than those in Section 5.1 in u, v variables. For an extension, we consider the case when α_{MH} depends on x_j, and solve

$$u_t - v_{xx} = 0,\ v \in \alpha_{MH}(x;u), \tag{69a}$$

$$v(\cdot,t) \in H_0^1(0,1) \text{ for } t > 0,\ u(x,0) \equiv const = \eta = 1.2. \tag{69b}$$

Here η exceeds a given maximum solubility v^*, and the unknowns evolve depending on that amount and on v^*. We consider three cases of a constant $v^* = v_c^*$, an affine $v^* = v_a^*$, and non-affine $v^* = v_n^*$,

TABLE 3. Convergence and iteration count for (69) for boundary condition cases: (a) constant, (b) affine, and (c) non-affine.

(a)

$1/h$	$1/\tau$	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
32	320	2	6.84e-03		9.58e-04		3.71e-03		6.31e-04		3.84e-03	
64	640	2	4.74e-03	0.530	5.05e-04	0.925	2.36e-03	0.654	3.36e-04	0.910	2.41e-03	0.672
128	1280	2	3.15e-03	0.586	2.57e-04	0.972	1.44e-03	0.713	1.73e-04	0.961	1.47e-03	0.717
256	2560	2	2.14e-03	0.560	1.28e-04	1.005	8.50e-04	0.760	8.55e-05	1.014	8.62e-04	0.768
512	5120	2	1.39e-03	0.623	6.04e-05	1.086	4.86e-04	0.806	4.05e-05	1.077	4.92e-04	0.810
16	1600	2	6.53e-03		7.15e-04		2.31e-03		2.85e-04		2.76e-03	
32	3200	2	4.28e-03	0.610	3.25e-04	1.138	7.12e-04	1.697	8.15e-05	1.807	1.17e-03	1.239
64	6400	2	2.93e-03	0.547	1.62e-04	1.009	3.48e-04	1.029	3.45e-05	1.239	6.03e-04	0.955
128	12800	2	1.98e-03	0.559	8.04e-05	1.005	2.17e-04	0.682	1.74e-05	0.986	3.33e-04	0.855
256	25600	2	1.31e-03	0.603	3.85e-05	1.063	1.31e-04	0.725	8.52e-06	1.033	1.81e-04	0.883
16	256	2	7.83e-03		1.15e-03		3.44e-03		6.38e-04		3.79e-03	
32	1024	2	4.39e-03	0.833	4.24e-04	1.436	1.31e-03	1.396	1.82e-04	1.811	1.55e-03	1.287
64	4096	2	2.69e-03	0.705	1.67e-04	1.343	4.88e-04	1.421	5.10e-05	1.834	6.57e-04	1.239

(b)

$1/h$	$1/\tau$	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
32	320	2	1.58e-02		1.83e-03		2.98e-03		4.56e-04		3.57e-03	
64	640	2	1.10e-02	0.515	9.46e-04	0.955	1.88e-03	0.665	2.39e-04	0.928	2.15e-03	0.729
128	1280	2	7.64e-03	0.529	4.75e-04	0.994	1.14e-03	0.718	1.22e-04	0.976	1.26e-03	0.768
256	2560	2	5.22e-03	0.551	2.33e-04	1.027	6.74e-04	0.762	6.00e-05	1.021	7.27e-04	0.798
512	5120	2	3.44e-03	0.602	1.09e-04	1.090	3.84e-04	0.810	2.83e-05	1.083	4.07e-04	0.838
16	1600	2	2.19e-02		2.95e-03		3.06e-03		4.29e-04		5.29e-03	
32	3200	2	1.48e-02	0.564	1.46e-03	1.016	1.17e-03	1.383	1.53e-04	1.488	2.68e-03	0.980
64	6400	2	1.04e-02	0.518	7.27e-04	1.003	5.08e-04	1.208	5.91e-05	1.371	1.37e-03	0.964
128	12800	2	7.11e-03	0.545	3.54e-04	1.039	2.47e-04	1.039	2.40e-05	1.297	6.94e-04	0.986
256	25600	2	4.69e-03	0.601	1.66e-04	1.090	1.29e-04	0.941	1.00e-05	1.263	3.45e-04	1.010
16	256	2	2.19e-02		3.16e-03		3.12e-03		5.72e-04		4.95e-03	
32	1024	2	1.43e-02	0.622	1.46e-03	1.113	1.30e-03	1.262	1.95e-04	1.552	2.57e-03	0.942
64	4096	2	9.35e-03	0.612	6.72e-04	1.120	5.52e-04	1.236	6.65e-05	1.552	1.29e-03	0.997

(c)

$1/h$	$1/\tau$	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
32	320	2	1.07e-02		1.22e-03		2.9e-03		4.75e-04		3.34e-03	
64	640	2	7.40e-03	0.533	6.33e-04	0.949	1.89e-03	0.656	2.53e-04	0.910	2.05e-03	0.706
128	1280	2	5.09e-03	0.539	3.19e-04	0.988	1.15e-03	0.717	1.29e-04	0.965	1.22e-03	0.751
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
16	1600	2	1.39e-02		1.61e-03		2.73e-03		3.57e-04		4.18e-03	
32	3200	2	9.50e-03	0.555	7.85e-04	1.040	1.00e-03	1.445	1.15e-04	1.635	2.04e-03	1.034
64	6400	2	6.61e-03	0.524	3.88e-04	1.016	4.35e-04	1.205	4.36e-05	1.400	1.04e-03	0.969
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
16	256	2	1.43e-02		1.86e-03		2.97e-03		5.30e-04		3.99e-03	
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

each satisfying $v^*(1) = 1$:

$$v_c^*(x) = 1, \tag{70}$$

$$v_a^*(x) = (1+x)/2, \tag{71}$$

$$v_n^*(x) = (1+2x-x^2)/2. \tag{72}$$

For these cases the convergence results are given in Table 3. The computed rates agree with the theory and are similar to those for Stefan problem. Additionally, the errors and convergence rates for the saturations S presented in Table 4 are similar to those for u.

TABLE 4. Convergence of saturations for (69) for boundary condition cases: constant, affine, and non-affine. In each case $1/\tau = 100/h$.

	constant				affine				non-affine			
$1/h$	$e_{s,2}$	$r_{s,2}$	$e_{s,1}$	$r_{s,1}$	$e_{s,2}$	$r_{s,2}$	$e_{s,1}$	$r_{s,1}$	$e_{s,2}$	$r_{s,2}$	$e_{s,1}$	$r_{s,1}$
16	6.16e-03		5.21e-04		1.67e-02		2.09e-03		1.11e-02		1.16e-03	
32	4.23e-03	0.542	2.65e-04	0.977	1.13e-02	0.563	1.04e-03	1.004	7.58e-03	0.546	5.82e-04	0.998
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

6. Conclusions

In this paper we analyzed a model and proposed a numerical scheme for evolution of methane hydrates. In addition, we considered other models of similar structure which include set–valued nonlinearities such as the Stefan problem. On one hand, we showed that one can extend monotone operator theory to cover the case when the graphs are parameter-dependent families such as in the underlying hydrate problem. On the other hand, we showed an efficient numerical solver for models with multivalued graphs using complementarity constraints and semismooth Newton methods. Both directions are important for future theoretical and applied developments. In particular, some work is underway on rigorous convergence estimates developed for general non-Lipschitz and parameter-dependent families of graphs α.

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