

CONTROL VOLUME APPROXIMATION OF DEGENERATE TWO PHASE POROUS FLOWS

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Abstract. Implicit Euler approximations of the equations governing the porous flow of two immiscible incompressible fluids are shown to be the Euler–Lagrange equations of a convex function. Tools from convex analysis are then used to develop robust fully discrete algorithms for their numerical approximation. Existence and uniqueness of solutions control volume approximations are established.

Key words. Degenerate, two phase flow, convexity

AMS subject classifications. 65N12, 76S05

1. Introduction. Numerical approximation of the equations modeling the flow of two incompressible immiscible fluids in a porous medium is considered. These equations take the form of conservation laws for the balance of mass of each fluid; letting ρ_π , $\pi = 1, 2$, denote the mass of each fluid per unit volume¹ of $\Omega \subset \mathbb{R}^d$,

$$\frac{\partial \rho_\pi}{\partial t} + \operatorname{div}(\rho_\pi \mathbf{v}_\pi) = q_\pi, \quad \text{in } (0, T) \times \Omega.$$

The velocities are determined from Darcy laws $\mathbf{v}_\pi = \hat{K}_\pi(\mathbf{b}_\pi - \nabla p_\pi)$ with body (gravity) forces \mathbf{b}_π , and the phase pressures p_π are determined from the incompressibility condition and a capillary pressure relation for the difference $p_1 - p_2$. Since the fluids are incompressible it is traditional to write $\rho_\pi = \tilde{\rho}_\pi s_\pi$ where $\tilde{\rho}_\pi$ is constant (the mass density of fluid π) and s_π is the saturation (volume of fluid π per unit volume of Ω).

These equations exhibit significant degeneracy in the spatial terms when one fluid is not present or displaces another ($\rho_\pi = 0$), or becomes immobile below a certain saturation ($\mathbf{v}_\pi = 0$). The incompressibility constraint gives rise to an additional degeneracy in the temporal term since the densities (ρ_1, ρ_2) are not a bijective function of the pressures (p_1, p_2) . In addition, if the porosity of the medium vanishes (or is small) in a portion of the domain Ω the densities ρ_π vanish.

Below it is shown that implicit Euler approximations of these equations can be cast as convex minimization problems. Implicit Euler approximations of the pair of equations (the simultaneous solution method [7]) were considered by Douglas et. al. [12] in 1959; however, to date the convex structure has not been exploited in the numerical context. The following statement from the survey article [19] by Rockafellar well illustrates the need to rectify this omission.

In fact the great watershed in optimization isn't between linearity and nonlinearity, but convexity and nonconvexity. Even for problems that aren't themselves of

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†Department of Mathematics, Carnegie Mellon University, Pittsburgh, PA 15213. Supported in part by National Science Foundation Grants DMS-1418991 and DREF-1729478. This work was also supported by the NSF through the Center for Nonlinear Analysis.

¹Frequently the density is defined to be mass per unit pore volume of Ω . This is poorly defined in regions where the pore volume vanishes (or is small).

convex type, convexity may enter, for instance, in setting up subproblems as part of an iterative numerical scheme.

Below tools from convex analysis are utilized to address the following fundamental issues.

- Existence and stability is established for a broad class of fully discrete schemes for the two phase problem.
- A detailed analysis of the control volume scheme is presented which for which the degeneracies can be completely characterized.
- Schemes for the minimization of degenerate convex problems are considered, and a numerical example presented.

1.1. Background. Porous flow of two imiscible incompressible fluids models the most easily implemented enhanced oil recovery process. For this reason these equations and their numerical simulation have been intensely studied in both the engineering and mathematical communities over the past half century giving rise to a vast body of literature on the topic. In this section we limit the scope of the discussion to the mathematical structure of these equations and the structural properties of numerical schemes associated with the degenerate nature of these problems. The text by Riviere [18] contains a concise synopsis of the two phase problem, and the monograph [7] provides a comprehensive introduction to both the physical models and numerical schemes for this problem.

Existence of solutions to the degenerate two phase problem were established by Kroner and Luckhaus [14] and Alt and DiBenedetto [1]. Essentially all existence results for this problem are established under the assumption that the permeability matrix \hat{K}_π of a phase only vanishes when the saturation of the phase vanishes (the partially degenerate case below). This precludes the situation where one phase can not completely displace the other [18]. A common approach for establishing existence of solutions is to observe that upon adding the equations for each phase the sum of the temporal derivatives vanishes since the fluids are incompressible. This gives an equation of the form

$$\operatorname{div} (s_1 \mathbf{v}_1 + s_2 \mathbf{v}_2) = q_1 + q_2.$$

It is frequently possible to introduce an enigmatic change of variables [1, 2, 5] to get $s_1 \mathbf{v}_1 + s_2 \mathbf{v}_2 = \lambda \nabla \mathbf{p}$, which results in an elliptic equation for (the “total pressure”) \mathbf{p} . The two phase problem can then be cast at an elliptic equation coupled to a parabolic problem, and this has spawned a corresponding class of numerical schemes numerical schemes [3, 6, 8, 17].

In order to circumvent degeneracies in the temporal term due to the incompressibility constraint it is frequently assumed that the fluids are slightly compressible for both the one and two phase problems, in the mathematical and numerical works e.g. [11, 13]. Posing the problem with saturations (densities) defined to be the volume (mass) of a phase per unit volume of Ω eliminates many of the difficulties associated with incompressibility. In this context the incompressibility constraint becomes $s_1 + s_2 = 1 - s_0$ where $s_0 : \Omega \rightarrow [0, 1]$ is the saturation of the medium [1, 21]. At points where $s_0(x) = 1$ it is immediate that $s_1 = s_2 = 0$ and the saturations are determined by the constraint. Numerical approximation of non-negative variables subject to linear constraints is a classical topic and are easily accommodated in this context.

2. Two Phase Problem. In this section the equations modeling the porous flow of two imiscible incompressible fluids are presented and their convexity properties developed. Degener-

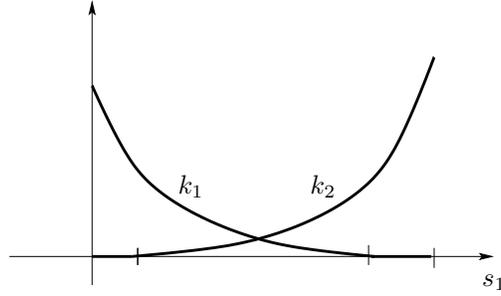


FIG. 2.1. Prototypical relative saturation curves.

acy can preclude rigorous derivations, so the presentation in this section is formal. In the next section finite dimensionality allows a rigorous treatment of control volume scheme.

2.1. Classical Formulation. When the fluids are incompressible, the mass per unit volume of the medium takes the form $\rho_\pi = \tilde{\rho}_\pi s_\pi$ where $\tilde{\rho}_\pi > 0$ is constant and $s_\pi = s_\pi(t, x)$ is the saturation; i.e. volume of fluid π per unit volume of Ω . The classical statement of the equations for the balance of mass for each phase then take the form

$$\frac{\partial s_\pi}{\partial t} - \operatorname{div} (K_\pi(\mathbf{s})(\nabla p_\pi - \mathbf{b}_\pi)) = 0, \quad (2.1)$$

where

- $K_\pi(\mathbf{s}) = s_\pi \hat{k}_\pi(\mathbf{s}) K_0 / \mu_\pi$, where K_0 is the symmetric positive semi-definite permeability matrix of the medium, μ_π is the viscosity and $\hat{k}_\pi(\mathbf{s}) = \hat{k}_\pi(x, \mathbf{s}) \geq 0$ is the relative permeability of phase π . The later characterizes the flow properties of the fluid when other fluids are present; Figure 2.1 illustrates prototypical curves for these coefficients. Note that $K_\pi = 0$ when $s_\pi = 0$ so degeneracy of the equations is unavoidable.
- \mathbf{b}_π are the external body forces (force per unit volume). Typically $\mathbf{b}_\pi = \rho_\pi \mathbf{g}$ where \mathbf{g} is the gravitational force per unit mass.
- The incompressibility constraint then becomes $s_0 + s_1 + s_2 = 1$, where $s_0 : \Omega \rightarrow [0, 1]$ is the saturation (volume ratio) of the medium so that $1 - s_0$ is the porosity. Also, implicit in this formulation are the constraints that the saturations must be non-negative.
- The phase pressures take the form $p_1 = p + p_c$ and $p_2 = p - p_c$ where p is the Lagrange multiplier dual to the incompressibility constraint, and $p_c = p_c(x, \mathbf{s})$ is the capillary pressure which characterizes the surface tension and wetting properties of the fluid.
- Equation (2.1) does not include terms modeling mass sources and sinks. Naive inclusion of a non-homogeneous term on the right hand side is not meaningful in the current setting since the left hand side vanishes in degenerate regions. Clearly solutions will not exist if, for example, a source term is introduced which extracts fluid from a region where none is present or injects fluid into a saturated impervious region.

In Section 4 we discuss the additional terms typically included in the mass balances (2.1) to model wells where fluids are injected and/or extracted and how their presence impacts the existence and uniqueness properties of the solutions.

NOTATION 2.1. Below $\mathbf{p} = (p_1, p_2)$ will denote the pair of pressures and $\mathbf{s} = (s_1, s_2)$ the pair of saturations.

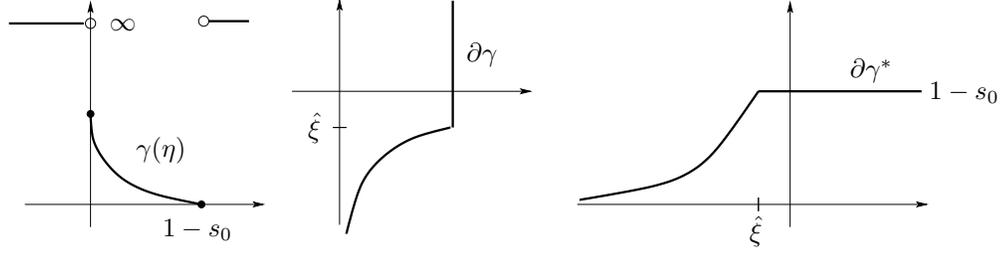


FIG. 2.2. Prototypical interfacial energy; $\eta \equiv (1 - s_0 + s_1 - s_2)/2 \in [0, 1 - s_0]$

2.2. Convex Structure. The capillary pressure is a monotone increasing function of the difference $s_1 - s_2$, so can be realized as the derivative of a convex² function of the difference, $p_c(\mathbf{s}) = \gamma'(s_1 - s_2)$. More generally, $p_\pi = p + \partial e_I / \partial s_\pi$ where $e_I = e_I(\mathbf{s})$ is a convex function modeling the energy (per unit volume of Ω) of the interfaces between the fluids (surface tension) and of the interfaces between the fluids and medium (wetting).

The pressure–saturation relation at each point $x \in \Omega$ can be written as $\mathbf{p} = \partial(I_L + \Gamma)(\mathbf{s})$, where $I_L, \Gamma : \mathbb{R}^2 \rightarrow \mathbb{R} \cup \{\infty\}$ are the convex functions $\Gamma(\mathbf{s}) = \gamma(s_1 - s_2)$ and

$$I_L(\mathbf{s}) = \begin{cases} 0 & s_1 + s_2 = 1 - s_0(x) \\ \infty & \text{otherwise} \end{cases} \quad \text{with } \gamma(s_1 - s_2) \equiv \begin{cases} \gamma(s_1 - s_2) & |s_1 - s_2| \leq 1 - s_0(x) \\ \infty & \text{otherwise,} \end{cases}$$

and $\partial(I_L + \Gamma)$ denotes the sub–gradient (at each point $x \in \Omega$). Here I_L is the indicator function of the set $L = \{\mathbf{s} \in \mathbb{R}^2 \mid s_1 + s_2 = 1 - s_0\}$ which enforces the equality constraint, and Γ is the sum of the surface tension function and the indicator of the set $\{\mathbf{s} \in \mathbb{R}^2 \mid |s_1 - s_2| \leq 1 - s_0\}$ which guarantees non–negativity of saturations on the set L .

Expanding the definition of the sub–gradient shows (see Figure 2.2)

$$\begin{pmatrix} p_1 \\ p_2 \end{pmatrix} \in p \begin{pmatrix} 1 \\ 1 \end{pmatrix} + (1/2)\partial\gamma(s_1 - s_2) \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

The inverse saturation–pressure relation is realized as $\mathbf{s} \in \partial(I_L + \Gamma)^*(\mathbf{p})$ where

$$(I_L + \Gamma)^*(\mathbf{p}) = \sup_{\mathbf{s} \in \mathbb{R}^2} (\mathbf{p} \cdot \mathbf{s} - (I_L + \Gamma)(\mathbf{s})),$$

is the convex conjugate of $I_L + \Gamma$. A calculation shows

$$\begin{pmatrix} s_1 \\ s_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 - s_0 \end{pmatrix} + (\gamma^*)'(p_1 - p_2) \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \quad (2.2)$$

For the porous flow problem γ is smooth on its domain, which is bounded, so γ^* is finite on all of the real line and is differentiable, $\partial\gamma^* = (\gamma^*)'$.

Example: A prototypical Brooks–Corey capillary pressure [4, 18] takes the form $p_c(\mathbf{s}) = -1/(2\sqrt{s_1})$. Note that $s_1 = (1 - s_0 + s_1 - s_2)/2 \equiv \eta$ when $s_0 + s_1 + s_2 = 1$. Then

$$\gamma(\eta) = \sqrt{1 - s_0} - \sqrt{\eta} + I_{[0, 1 - s_0]}(\eta), \quad \partial\gamma(\eta) = \begin{cases} \frac{-1}{2\sqrt{\eta}} & \eta \in (0, 1 - s_0) \\ \left[\frac{-1}{2\sqrt{1 - s_0}}, \infty \right) & \eta = 1 - s_0, \end{cases}$$

²In the engineering literature the capillary pressure takes the opposite sign. With the choice of sign utilized here p_c can be realized as the derivative of a convex rather than a concave function.

where $I_{[0,1-s_0]}$ is the indicator function of the interval $[0, 1 - s_0]$. The conjugate function and its derivative are

$$\gamma^*(\xi) = \begin{cases} -\sqrt{1-s_0} - \frac{1}{4\xi} & \xi \in \left(-\infty, \frac{-1}{2\sqrt{1-s_0}}\right] \\ (1-s_0)\xi & \xi \in \left[\frac{-1}{2\sqrt{1-s_0}}, \infty\right), \end{cases} \quad \partial\gamma^*(\xi) = \begin{cases} \frac{1}{4\xi^2} & \xi \in \left(-\infty, \frac{-1}{2\sqrt{1-s_0}}\right] \\ 1-s_0 & \xi \in \left[\frac{-1}{2\sqrt{1-s_0}}, \infty\right). \end{cases}$$

These functions take the form shown in Figure 2.2. In general $s_0 = s_0(x)$ so γ may depend explicitly upon $x \in \Omega$. Since this does not influence the analysis below the dependence upon x will not be exhibited in the notation. \square

Using equations (2.2) to eliminate the saturations from equations (2.1) gives a coupled pair of degenerate diffusion equations for the pressures. Initial data for these equations would be the saturations at time $t = 0$, and the natural no-flux boundary conditions take the form $K_\pi \nabla p_\pi = K_\pi \mathbf{b}_\pi$. Under mild regularity assumptions, the chain rule for sub-gradients [23] states that

$$\mathbf{p} \in \partial(I_L + \Gamma)(\mathbf{s}) \quad \Rightarrow \quad (\mathbf{s}_t, \mathbf{p}) = \frac{d}{dt}(I_L + \Gamma)^*(\mathbf{p}),$$

so the natural a-priori estimate for equations (2.1)–(2.2) with no-flux boundary data is

$$\int_\Omega \gamma^*(\mathbf{p}(t)) + \int_0^t \int_\Omega \sum_{\pi=1}^2 |\nabla p_\pi|_{K_\pi}^2 = \int_\Omega \gamma^*(\mathbf{p}(0)) + \int_0^t \int_\Omega \sum_{\pi=1}^2 (\mathbf{b}_\pi, \nabla p_\pi)_{K_\pi}. \quad (2.3)$$

Here $(\mathbf{p}, \mathbf{q})_{K_\pi} = K_\pi \mathbf{p} \cdot \mathbf{q}$ is the semi-inner product on pairs induced by K_π , and we write $\gamma^*(\mathbf{p}) \equiv \gamma^*(p_1 - p_2)$.

2.3. Implicit Euler Approximation. Letting $\tau > 0$ denote a time step, the implicit Euler approximation of equations (2.1) and (2.2) becomes

$$s_\pi^n - s_\pi^{n-1} - \tau \operatorname{div} (K_\pi^{n-1} (\nabla p_\pi^n - \mathbf{b}_\pi^{n-1})) = 0, \quad \mathbf{s}^n \in \partial(I_L + \Gamma)^*(\mathbf{p}^n). \quad (2.4)$$

In these expressions the superscript indicates the temporal index, $s_\pi^n \simeq s_\pi(n\tau)$ and $K_\pi^{n-1} = K_\pi(\mathbf{s}^{n-1})$. Solutions of this scheme with no-flux boundary conditions are minimizers of

$$\Psi(\mathbf{p}) = \int_\Omega \left\{ \gamma^*(p_1 - p_2) - s_1^{n-1}(p_1 - p_2) + \frac{\tau}{2} \sum_{\pi=1}^2 |\nabla p_\pi - \mathbf{b}_\pi^{n-1}|_{K_\pi^{n-1}}^2 \right\}. \quad (2.5)$$

Convexity of γ^* guarantees

$$(\gamma^*)'(p_1^n - p_2^n) ((p_1^n - p_2^n) - (p_1^{n-1} - p_2^{n-1})) \geq \gamma^*(p_1^n - p_2^n) - \gamma^*(p_1^{n-1} - p_2^{n-1}),$$

from which the discrete analog of (2.3) for solutions of of the implicit Euler scheme (2.4) follows,

$$\int_\Omega \gamma^*(\mathbf{p}^n) + \tau \sum_{m=1}^n \int_\Omega \sum_{\pi=1}^2 |\nabla p_\pi^m|_{K_\pi^{m-1}}^2 \leq \int_\Omega \gamma^*(\mathbf{p}^0) + \tau \sum_{m=1}^n \int_\Omega \sum_{\pi=1}^2 (\nabla p_\pi^m, \mathbf{b}_\pi^{m-1})_{K_\pi^{m-1}}.$$

2.4. Degeneracy. The natural space of functions for which $\Psi(\mathbf{p})$ is finite is

$$U^{n-1} = \{\mathbf{p} \in L^1(\Omega)^2 \mid \int_{\Omega} \sum_{\pi=1}^2 |\nabla p_{\pi}|_{K_{\pi}^{n-1}}^2 < \infty\};$$

however, while the permeabilities K_{π}^{n-1} are typically bounded they may vanish on large subsets of Ω . In particular, the spatial term in Ψ is not strictly convex so minimizers are not unique; for example, p_{π} is undefined when a phase vanishes. In addition, properties typically available for Sobolev functions, such as trace theorems, are not available. Non-uniqueness also arises due to the no-flux boundary condition and saturation of the pores by one fluid; specifically,

1. $\Psi(\mathbf{p})$ is unchanged upon shifting both pressures by the same constant, $(p_1, p_2) \mapsto (p_1 + c, p_2 + c)$. As for the classical Neumann problem, this degeneracy may be eliminated by working on the subspace of functions for which the average of $p_1 + p_2$ vanishes.
2. If $\hat{\xi} = \hat{\xi}(x) \in \mathbb{R}$ is the first point where $(\gamma^*)'(\xi)$ attains its maximal value of $1 - s_0$, the pressure difference $p_1 - p_2$ is not determined by the surface tension when $p_1 - p_2 - \hat{\xi} \geq 0$. Specifically, increasing p_1 or decreasing p_2 does not change the first terms in the formula of Ψ ,

$$\gamma^*(p_1 - p_2) - s_1^{n-1}(p_1 - p_2) = \gamma^*(p_1 + c - p_2) - s_1^{n-1}(p_1 + c - p_2), \quad c \geq 0,$$

since the derivative of $\xi \mapsto \gamma^*(\xi) - s_1^{n-1}\xi$ is constant when $\xi \geq \hat{\xi}$. Setting $\Omega_{\pi}^{n-1} = \{x \in \Omega \mid K_{\pi}^{n-1}(x) = 0\}$ and $\Omega_0^{n-1} = \Omega_1^{n-1} \cup \Omega_2^{n-1}$ it follows that

$$\tilde{\Psi}(\mathbf{p}) \equiv \Psi(\mathbf{p}) + \int_{\Omega_0^{n-1}} (1/2) \max(0, p_1 - p_2 - \hat{\xi})^2 \quad (2.6)$$

has the same minima as Ψ and at a minimum $p_2 - p_1 = \hat{\xi}$ on the degenerate sets.

For the example illustrated in Figure 2.2 the slope at the origin is infinite, $\gamma'(0) = -\infty$, so $(\gamma^*)'(\xi) > 0$ on $(-\infty, \hat{\xi})$. If $\gamma'(0)$ were finite then $(\gamma^*)'(\xi)$ would also vanish on an interval of the form $(-\infty, \hat{\xi})$, and a term of the form $\min(0, p_1 - p_2 + \hat{\xi})^2$ would provide a selection of the pressures on the degenerate sets.

3. If $s_0 = 1$ in a subset of the domain then $\gamma^*(\xi) = 0$, $s_1 = s_2 = 0$, and both equations for the balance of mass degenerate to zero. Since s_0 is assumed known a-priori this case can be eliminated by excising these points from the domain; $\Omega \mapsto \Omega \setminus \bar{\Omega}_0$ where $\Omega_0 = \{x \in \Omega \mid s_0(x) = 1\}$. Below we assume that $s_0 < 1$; however, in a numerical context it may be inconvenient to triangulate $\Omega \setminus \bar{\Omega}_0$ in which case a term of the form $\int_{\Omega_0} p_1^2 + p_2^2$ can be included to eliminate this degeneracy.

In the fully discrete setting existence and uniqueness of minimizers of control volume approximations of $\tilde{\Psi}$ are established.

2.5. Degenerate Convex Minimization. While the implicit Euler approximation of the two phase problem is degenerate it is not singular. Specifically, Ψ_h and $\tilde{\Psi}_h$ have Lipschitz gradients, and minimizing such functions has, and continues to be, intensely studied in the optimization community. The numerical examples below utilize the preconditioned Nesterov algorithm with properties summarized in the following theorem.

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SEMI-SMOOTH NEWTON( $u_0$ )
Initialize:  $\beta = 1$ ,  $\epsilon = 10^{-8}$ ,  $u = u_{old} = u_0$ ,  $\psi_{old} = \psi(u) + 1$ .
while ( $|\nabla\psi(u)| > \epsilon$ )
  if ( $\psi(u) > \psi_{old}$ )
     $\beta = \beta/2$ 
    if ( $\beta < \epsilon$ ) then return (FAIL)
     $u = u_{old} - \beta\delta u$ 
  else
     $\psi_{old} = \psi(u)$ ,  $u_{old} = u$ 
    Solve  $(D^2\psi(u) + \epsilon I)\delta u = \nabla\psi(u)$ 
     $u = u - \beta\delta u$ 
     $\beta = \min(1, 1.25\beta)$ 
return ( $u$ )

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FIG. 2.3. Semi-Smooth Newton scheme for solving $\nabla\psi(u) = 0$.

THEOREM 2.2 (Nesterov). Let U be a Hilbert space with Reisz map $\mathcal{R} : U \rightarrow U'$ and let $\psi : U \rightarrow \mathbb{R}$ be convex and satisfy

$$(\nabla\psi(v) - \nabla\psi(u), v - u)_U \leq \|v - u\|_U^2. \quad (2.7)$$

Define the sequence of real numbers $\{\gamma_n\}_{n=0}^\infty$ by

$$\gamma_n = \frac{1 - \lambda_n}{\lambda_{n+1}}, \quad \text{where } \lambda_0 = 0 \quad \text{and} \quad \lambda_n = \frac{1 + \sqrt{1 + 4\lambda_{n-1}^2}}{2}, \quad n = 1, 2, \dots,$$

and given $u_1 \in U$ define the sequences $\{v_n\}_{n=1}^\infty$ and $\{u_n\}_{n=1}^\infty \subset U$ by $v_1 = u_1$ and

$$v_{n+1} = u_n - g_n, \quad u_{n+1} = (1 - \gamma_n)v_{n+1} + \gamma_nv_n, \quad \text{with } \mathcal{R}g_n = \nabla\psi(u_n).$$

If $\psi(u_*) = \inf_{u \in U} \psi(u)$ then

$$\psi(v_n) - \psi(u_*) \leq \frac{2\|u_1 - u_*\|_U^2}{n^2} \quad \text{and} \quad \|g_n\|_U \leq \frac{4\|u_1 - u_*\|_U}{n}.$$

The algorithm in this theorem requires inversion of the Reisz map which, in the finite dimensional context, requires a single LU decomposition of the “stiffness” matrix associated with the inner product $(\cdot, \cdot)_U$. The convex function Ψ in equation (2.5) is quadratic in the spatial terms in which case a norm with inner product satisfying the hypothesis (2.7) is

$$\|\mathbf{p}\|_U^2 = \int_\Omega \frac{\beta}{2}(p_1 - p_2)^2 + \frac{\tau}{2} \sum_{\pi=1}^2 |\nabla p_\pi|_{K_\pi^{n-1}}^2,$$

where β is a bound on the second derivative of γ^* .

The preconditioned Nesterov algorithm is robust and the initial iterates have good descent properties, so we use it to obtain a good initial guess for the Newton like scheme in Figure 2.3 when more than a few decimal digits are required. This semi-smooth Newton scheme uses a selection from the Hessian to compute a Newton descent direction which is then scaled to achieve descent.

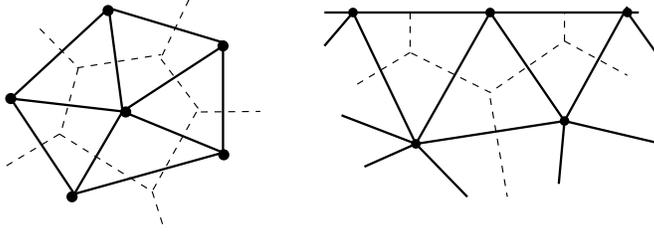


FIG. 3.1. Voronoi regions of interior (left) and boundary (right) nodes.

3. Spatial Approximation. Utilizing a finite dimensional space of functions for the pressures in equation (2.4) gives a fully discrete approximation of the two phase porous flow problem (2.1)–(2.2). Since the continuity properties of the pressures are problem dependent, and may vary with time, spaces which admit discontinuous solutions are natural candidates. In order to focus on the issues that arise with the degeneracies we assume that the permeability matrices K_π are diagonal and consider the control volume scheme with piecewise constant pressures. This scheme inherits stability estimates identical in structure to those presented for the continuous problem in Section 2.3.

3.1. Control Volume Scheme. Given a Delaunay triangulation, \mathcal{T}_h , of the domain $\Omega \subset \mathbb{R}^3$, the control volumes are taken to be the Voronoi regions in Ω associated with each node³ of \mathcal{T}_h . The Voronoi edges/faces (2d/3d) bisect, and are perpendicular to, the edges of \mathcal{T}_h , and the vertices of the Voronoi regions are the circumcenters of the triangles/tetrahedra containing the node. We assume that the circum circles/spheres of the edges/triangles on the boundary of Ω do not contain any nodes in their interior so that the Voronoi regions of nodes on the boundary are well formed [20]; see Figure 3.1.

Integrating equation (2.1) over a Voronoi cell C_i corresponding to a node of \mathcal{T}_h indexed by i , shows

$$\int_{C_i} (s_\pi^n - s_\pi^{n-1}) - \tau \int_{\partial C_i} K_\pi^{n-1} (\nabla p_\pi - \mathbf{b}_\pi) \cdot \mathbf{n} = 0, \quad \pi = 1, 2.$$

Letting \mathcal{N}_i denote the set of nodes connected to i by an edge in \mathcal{T}_h , and assuming that $K_\pi = k_\pi I$ is diagonal, and approximating the integrals with one point quadrature rules and derivatives by differences [15, 16] gives

$$|C_i| (s_{\pi i}^n - s_{\pi i}^{n-1}) + \tau \sum_{j \in \mathcal{N}_i} \frac{A'_{ij} k_{\pi ij}^{n-1}}{h_{ij}} \left(p_{\pi i}^n - p_{\pi j}^n + h_{ij} \mathbf{b}_{\pi ij}^{n-1} \cdot \mathbf{n}_{ij} \right) = 0. \quad (3.1)$$

In this expression h_{ij} is the length of the edge from node i to node j , A'_{ij} the area/length of the dual Voronoi face/edge in 3d/2d, and $k_{\pi ij}^{n-1}$ and $\mathbf{b}_{\pi ij}^{n-1}$ are the averages of the permeabilities and body forces at the two nodes, and \mathbf{n}_{ij} the unit outward vector parallel to the edge. Equation (2.2) is used to compute the saturations \mathbf{s}_i from the pressures \mathbf{p}_i at each node.

Letting \mathcal{N}_h denote the node set and \mathcal{E}_h the edge set of \mathcal{T}_h , equations (3.1) are the Euler Lagrange

³We refer to the points of the triangulation as *nodes* to avoid confusion with the *vertices* of the graph constructed below.

equations of the convex function $\Psi_h : \mathbb{R}^{|\mathcal{N}_h|} \times \mathbb{R}^{|\mathcal{N}_h|} \rightarrow \mathbb{R}$ given by

$$\begin{aligned} \Psi_h(\mathbf{p}) = & \sum_{i \in \mathcal{N}_h} |C_i| (\gamma^*(p_{1i} - p_{2i}) - s_{1i}^{n-1}(p_{1i} - p_{2i})) \\ & + \frac{\tau}{2} \sum_{(i,j) \in \mathcal{E}_h} \frac{A'_{ij}}{h_{ij}} \sum_{\pi=1}^2 k_{\pi ij}^{n-1} \left(p_{\pi i} - p_{\pi j} + h_{ij} \mathbf{b}_{\pi ij}^{n-1} \cdot \mathbf{n}_{ij} \right)^2, \end{aligned}$$

which is the discrete analog of the function Ψ in equation (2.5). Solutions of the control volume (3.1) scheme satisfy the stability estimate

$$\begin{aligned} \sum_{i \in \mathcal{N}_h} |C_i| \gamma^*(\mathbf{p}_i^n) + \tau \sum_{m=1}^n \sum_{(i,j) \in \mathcal{E}_h} \frac{A'_{ij}}{h_{ij}} \sum_{\pi=1}^2 k_{\pi ij}^{n-1} (p_{\pi i}^m - p_{\pi j}^m)^2 \leq & \sum_{i \in \mathcal{N}_h} |C_i| \gamma^*(\mathbf{p}_i^0) \\ & + \tau \sum_{m=1}^n \sum_{(i,j) \in \mathcal{E}_h} \frac{A'_{ij}}{h_{ij}} \sum_{\pi=1}^2 k_{\pi ij}^{m-1} (p_{\pi i}^m - p_{\pi j}^m) h_{ij} \mathbf{b}_{\pi ij}^{m-1} \cdot \mathbf{n}_{ij}. \end{aligned}$$

As for the continuous problem, Ψ_h is invariant under translation $(p_1, p_2) \mapsto (p_1 + c, p_2 + c)$ for $c \in \mathbb{R}$. For the prototypical interfacial energy illustrated in Figure 2.2, the arguments in Section 2.4 for the continuous problem apply verbatim to the current setting to show that the function

$$\tilde{\Psi}_h(\mathbf{p}) = \Psi_h(\mathbf{p}) + \sum_{i \in \mathcal{N}_{0h}^{n-1}} |C_i| \max(0, p_{1i} - p_{2i} - \hat{\xi}_i)^2, \quad (3.2)$$

has the same minimum as Ψ_h , where $\mathcal{N}_{0h}^{n-1} = \mathcal{N}_{1h}^{n-1} \cup \mathcal{N}_{2h}^{n-1}$ with $\mathcal{N}_{\pi h}^{n-1} = \{i \mid k_{\pi ij}^{n-1} = 0, j \in \mathcal{N}_i\}$, and $\hat{\xi}_i$ is the first point where $(\gamma^*)'(\xi_i) = 1 - s_0(x_i)$.

3.2. Existence of Solutions. In this section solutions of the control volume scheme (3.1) are constructed as minima of $\tilde{\Psi}_h$. Since $\tilde{\Psi}_h$ is convex on a finite dimensional space existence follows from the coercivity condition $\lim_{|\mathbf{p}| \rightarrow \infty} \tilde{\Psi}_h(\mathbf{p}) = \infty$; equivalently, a bound on $\tilde{\Psi}_h(\mathbf{p})$ implies \mathbf{p} is bounded. Coercivity will be established under the following assumptions which characterize the prototypical interfacial energies and permiabilities illustrated in Figures 2.1 and 2.2, and the meshes illustrated in Figure 3.1.

ASSUMPTION 3.1. $\Omega \subset \mathbb{R}^d$ is a bounded connected domain.

- $s_0 : \Omega \rightarrow [0, 1]$; specifically, $s_0(x) < 1$ for all $x \in \Omega$.
- There exists $C > 0$ such that the permiabilities $k_\pi : \Omega \times [0, 1] \rightarrow \mathbb{R}$ satisfy $0 \leq k_\pi(x, s_\pi) \leq C$ and $k_\pi(x, 0) = 0$. In addition,

$$k_1(x, s_1) + k_2(x, s_2) > 0 \quad \text{when} \quad s_1 + s_2 = 1 - s_0(x).$$

- For each $x \in \Omega$ there exists $\hat{\xi}(x) \in \mathbb{R}$ such that $\gamma^*(x, \cdot) : \mathbb{R} \rightarrow \mathbb{R}$ is convex with derivative strictly increasing on $(-\infty, \hat{\xi}(x))$, and

$$\lim_{\xi \rightarrow -\infty} (\gamma^*)'(x, \xi) = 0, \quad \text{and} \quad (\gamma^*)'(x, \xi) = 1 - s_0(x), \quad \xi \geq \hat{\xi}(x).$$

- \mathcal{T}_h is a Delaunay triangulation of Ω and the circumballs of boundary simplices do not contain any nodes in their interiors.

THEOREM 3.2. *Let the domain, coefficients, and triangulation satisfy Assumptions 3.1 and $\tilde{\Psi}_h : \mathbb{R}^{|\mathcal{N}_h|} \times \mathbb{R}^{|\mathcal{N}_h|} \rightarrow \mathbb{R}$ be the convex function in equation (3.2). Then $\tilde{\Psi}_h$ is coercive on $\{\mathbb{R}^{|\mathcal{N}_h|} \times \mathbb{R}^{|\mathcal{N}_h|} \rightarrow \mathbb{R} \mid \sum_{i \in \mathcal{N}_h} |C_i|(p_{1i} + p_{2i}) = 0\}$; in particular, minimizers of $\tilde{\Psi}_h$ exist.*

Proof. Fix $M > 0$ and let $\mathbf{p} : \mathbb{R}^{|\mathcal{N}_h|} \times \mathbb{R}^{|\mathcal{N}_h|} \rightarrow \mathbb{R}$ satisfy $\tilde{\Psi}_h(\mathbf{p}) \leq M$. Assumptions 3.1 guarantee that the function $\xi \mapsto \gamma^*(\xi) - s_1^{n-1}\xi$ is bounded below, and since the other terms forming $\tilde{\Psi}_h$ are non-negative the bound upon $\tilde{\Psi}_h(\mathbf{p})$ implies bounds upon each of them. Specifically, each of the terms

1. $\sum_{i \in \mathcal{N}_h} |C_i| (\gamma^*(p_{1i} - p_{2i}) - s_1^{n-1}(p_{1i} - p_{2i}))$
2. $\sum_{i \in \mathcal{N}_{2h}^{n-1}} |C_i| \max(0, p_{1i} - p_{2i} - \hat{\xi}_i)^2$, and
3. $\sum_{(i,j) \in \mathcal{E}_h} \frac{A'_{ij}}{h_{ij}} k_{\pi ij}^{n-1} (p_{\pi i} - p_{\pi j})^2$, with $\pi = 1$ and 2 ,

are bounded. Below we show that these bounds guarantees a bound on the differences $p_{1i} - p_{2i}$ for all $i \in \mathcal{N}_h$. Granted this, the elementary identities

$$\begin{aligned} |p_{1i} - p_{1j}| &\leq |p_{1i} - p_{2i}| + |p_{2i} - p_{2j}| + |p_{2j} - p_{1j}| \\ |p_{2i} - p_{2j}| &\leq |p_{2i} - p_{1i}| + |p_{1i} - p_{1j}| + |p_{1j} - p_{2j}| \end{aligned}$$

show that the semi-norm

$$|\mathbf{p}|^2 \equiv \sum_{i \in \mathcal{N}_j} |C_i| |p_{1i} - p_{2i}| + \tau \sum_{\pi=1}^2 \sum_{(i,j) \in \mathcal{E}_h} \frac{A'_{ij}}{h_{ij}} (k_{1ij}^{n-1} + k_{2ij}^{n-1}) (p_{\pi i} - p_{\pi j})^2$$

is bounded by a constant depending only upon $M = \tilde{\Psi}_h(\mathbf{p})$. Under the assumptions Ω is connected and $k_1 + k_2 > 0$ the discrete Poincare inequality shows that this is a norm on the subspace $\{\mathbf{p} : \mathbb{R}^{|\mathcal{N}_h|} \times \mathbb{R}^{|\mathcal{N}_h|} \rightarrow \mathbb{R} \mid \sum_{i \in \mathcal{N}_h} |C_i|(p_{1i} + p_{2i}) = 0\}$, and coercivity follows.

To establish a bound upon the differences $p_{1i} - p_{2i}$ we consider the two cases, $0 < s_{1i}^{n-1} < 1 - s_0(x_i)$ and $s_{1i}^{n-1} = 1 - s_0(x_i)$. Note that $s_1 = (\gamma^*)'(p_1 - p_2) > 0$, so these two cases are exhaustive.

- If $0 < s_{1i}^{n-1} < 1 - s_0(x_i)$ Assumptions 3.1 show

$$\lim_{\xi \rightarrow -\infty} \frac{d}{d\xi} (\gamma^*(\xi) - s_{1i}^{n-1}\xi) = -s_{1i}^{n-1} \quad \text{and} \quad \lim_{\xi \rightarrow \infty} \frac{d}{d\xi} (\gamma^*(\xi) - s_{1i}^{n-1}\xi) = 1 - s_0(x_i) - s_{1i}^{n-1}.$$

It follows that $\xi \mapsto \gamma^*(\xi) - s_{1i}^{n-1}\xi$ has linear growth at $\pm\infty$ so is coercive.

- If $s_{1i}^{n-1} = 1 - s_0(x_i)$ then $\gamma^*(\xi) - s_{1i}^{n-1}\xi$ has linear growth at $-\infty$ so a bound on this term bounds the difference $p_{1i} - p_{2i}$ below by a (typically negative) constant. In addition $s_{2i}^{n-1} = 0$ so $k_2(s_{2i}^{n-1}) = 0$ and $k_1(s_{1i}^{n-1}) > 0$ so $k_{1ij}^{n-1} > 0$ for each $j \in \mathcal{N}_i$.

To bound the pressure differences above we consider the two cases:

- If $k_{2ij}^{n-1} = 0$ for all $j \in \mathcal{N}_i$ then $i \in \mathcal{N}_{2h}^{n-1}$ and the pressure difference is bounded above by $\max(0, p_{1i} - p_{2i} - \hat{\xi}_i)^2$.
- If $k_{2ij}^{n-1} > 0$ for some $j \in \mathcal{N}_i$ then $s_{2j}^{n-1} > 0$ so $s_{1j}^{n-1} < 1 - s_0(x_j)$ and the previous case then bounds $p_{1j} - p_{2j}$. The elementary identity

$$|p_{1i} - p_{2i}| \leq |p_{1i} - p_{1j}| + |p_{1j} - p_{2j}| + |p_{2j} - p_{2i}|$$

provides a bound on $p_{1i} - p_{2i}$ since $k_{1ij}^{n-1} > 0$ and $k_{2ij}^{n-1} > 0$.

□

Note that this argument only requires the additional term in $\tilde{\Psi}_h$ to include the sum over $i \in \mathcal{N}_{2h}^{n-1}$; summing over $\mathcal{N}_{0h}^{n-1} = \mathcal{N}_{1h}^{n-1} \cup \mathcal{N}_{2h}^{n-1}$ is required for the uniqueness arguments below.

3.3. Uniqueness of Minimizers. In this section it is shown that in many instances the additional terms included in $\tilde{\Psi}_h$ are sufficient to select a unique minimum of Ψ_h . While all minima are solutions of the control volume scheme (3.1), and uniqueness is not required by the minimization algorithms presented in Section 2.5, elimination of degeneracy in a numerical context and repeatability of numerical computations is desirable.

To establish uniqueness we consider two minimizers \mathbf{p} and $\tilde{\mathbf{p}}$ of $\tilde{\Psi}_h$. Expanding the identity

$$0 = \tilde{\Psi}_h(\mathbf{p}) + \tilde{\Psi}_h(\tilde{\mathbf{p}}) - 2\tilde{\Psi}_h\left(\frac{1}{2}(\mathbf{p} + \tilde{\mathbf{p}})\right),$$

which follows from convexity of the set of minimizers, shows

$$\begin{aligned} 0 &= \sum_{i \in \mathcal{N}_h} |C_i| \left(\gamma^*(\xi_i) + \gamma^*(\tilde{\xi}_i) - 2\gamma^*\left(\frac{1}{2}(\xi_i + \tilde{\xi}_i)\right) \right) \\ &\quad + \frac{\tau}{4} \sum_{(i,j) \in \mathcal{E}_h} \frac{A'_{ij}}{h_{ij}} \sum_{\pi=1}^2 k_{\pi ij}^{n-1} \left((p_{\pi i} - \tilde{p}_{\pi i}) - (p_{\pi j} - \tilde{p}_{\pi j}) \right)^2 \\ &\quad + \sum_{i \in \mathcal{N}_{0h}^{n-1}} |C_i| \left(\max(0, \xi_i - \hat{\xi}_i)^2 + \max(0, \tilde{\xi}_i - \hat{\xi}_i)^2 - 2 \max(0, \frac{1}{2}(\xi_i + \tilde{\xi}_i) - \hat{\xi}_i)^2 \right), \end{aligned} \quad (3.3)$$

where $\xi_i = p_{1i} - p_{2i}$ and $\tilde{\xi}_i = \tilde{p}_{1i} - \tilde{p}_{2i}$. Note that each summand may be identified as a difference quotient for a second derivative for a convex function, so is non-negative. That each term vanishes is useful at nodes where the term is strictly convex; at nodes where γ^* has linear growth it is necessary to directly compare $\tilde{\Psi}_h(\mathbf{p})$ and $\tilde{\Psi}_h(\tilde{\mathbf{p}})$.

The following definitions characterize the regions where the spatial terms for each pressure are strictly convex, and their overlap.

DEFINITION 3.3. *Let \mathcal{T}_h be a triangulation of a domain $\Omega \subset \mathbb{R}^d$ and for $\pi = 1, 2$ let $k_\pi : \mathcal{N}_h \rightarrow [0, \infty)$ be non-negative functions on the node set of \mathcal{T}_h , $\pi = 1, 2$.*

- *Two nodes of \mathcal{T}_h are k_π -connected if there is a path in the edge set of \mathcal{T}_h which does not contain two consecutive nodes for which k_π vanishes.*
- *A k_π -component of \mathcal{N}_h is an equivalence class of the equivalence relation k_π -connectedness.*
- *The non-trivial k_π -components are those which contain at least one node $v \in \mathcal{N}_h$ for which $k_\pi(v) > 0$, and the set of these components is denoted by \mathcal{V}_π .*
- *The overlap graph, G corresponding to k_1 and k_2 is the graph with vertex set $\mathcal{V}_1 \cup \mathcal{V}_2$, and (V_1, V_2) is in the edge set of G if and only if $V_1 \cap V_2 \neq \emptyset$.*

Note that each \mathcal{V}_π is a disjoint partition of a subset of \mathcal{N}_h , so an edge in G necessarily has one vertex in \mathcal{V}_1 and one in \mathcal{V}_2 , so G is bipartite, and vertices $V_\pi \in \mathcal{V}_\pi$ are connected in the sense that for each pair of nodes $m, n \in V_\pi$ there is path in the edge set of \mathcal{T}_h from m to n containing vertices in V_π . Figure 3.2 illustrates the bipartite structure of G where two copies of Ω are represented by the upper and lower lines with each partitioned into components and degenerate regions \mathcal{N}_{1h}^{n-1} and \mathcal{N}_{2h}^{n-1} . A key observation is that adding a constant to all the pressures $p_{\pi i}$ in a component $V_\pi \in \mathcal{V}_\pi$ does not change middle (gradient) term in equation (3.3); coupling with the other component of the pressure is through the interfacial energy γ^* .

The following elementary properties of intersecting components will be used below.

LEMMA 3.4. *Let \mathcal{T}_h be a triangulation of a domain $\Omega \subset \mathbb{R}^d$ with node set \mathcal{N}_h , and G be the overlap graph of two functions $k_\pi : \mathcal{N}_h \rightarrow [0, \infty)$ for which $k_1(n) + k_2(n) > 0$ for every $n \in \mathcal{N}_h$.*

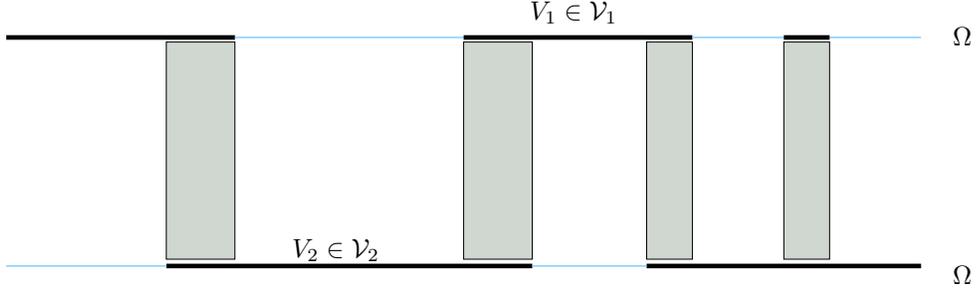


FIG. 3.2. Diagram of the graph G . Heavy lines indicate components in \mathcal{V}_1 (upper) and \mathcal{V}_2 (lower) and light lines the degenerate regions. Gray areas indicate overlap of non-trivial components.

1. If (V_1, V_2) is an edge in G , then for $\pi = 1, 2$ there exists $n_\pi \in V_1 \cap V_2$ such that $k_\pi(n_\pi) > 0$.
2. If Ω is connected then G is connected.

Proof.

1. By symmetry it suffices to show there exists $m \in V_1 \cap V_2$ with $k_2(m) > 0$. If $V_2 \subset V_1$ the result is immediate since, being non-degenerate, V_2 contains a vertex with this property. Otherwise, there exists $m' \in V_1 \cap V_2$ and $n' \in V_2 \setminus V_1$, and since V_2 is edge-connected in \mathcal{T}_h there exists an edge (m, n) of \mathcal{T}_h on a path from m' to n' in V_2 for which $m \in V_1 \cap V_2$ and $n \in V_2 \setminus V_1$. Then $k_1(m) = 0$ since $n \in V_1$ otherwise, so $k_2(m) = k_1(m) + k_2(m) > 0$ by hypothesis.
2. When Ω is connected it is immediate that the nodes of the triangulation are edge connected in \mathcal{T}_h . If $V_\pi, V_{\pi'} \in \mathcal{V}_1 \cup \mathcal{V}_2$ are vertices of G , let $n_\pi \in V_\pi$ and $n_{\pi'} \in V_{\pi'}$ be nodes of \mathcal{T}_h . Since \mathcal{T}_h is edge-connected there exists a path from n_π to $n_{\pi'}$ in the edge set of \mathcal{T}_h . Whenever this path exits a component, say $U_1 \in \mathcal{V}_1$, there is an edge (m_1, m_2) of \mathcal{T}_h with $m_1 \in U_1$ and $m_2 \notin U_1$ in which case $k_1(m_2) = 0$, so $k_2(m_2) > 0$ whence m_2 is in a non-degenerate component $m_2 \in U_2 \in \mathcal{V}_2$. In addition, since $k_2(m_2) > 0$ it follows that $m_1 \in U_2$, so $m_1 \in U_1 \cap U_2$ hence (U_1, U_2) is an edge in G . Chaining together all such edges in G gives a path in G from V_π to $V_{\pi'}$.

□

COROLLARY 3.5. *Let the permittivities k_π , interfacial energy γ , and triangulation satisfy Assumptions 3.1, and let $k_\pi^{n-1} : \mathcal{N}_h \rightarrow \mathbb{R}$ be the functions with values $k_\pi^{n-1} = k_\pi(s_\pi^{n-1})$. Let \mathcal{V}_π be the sets of non-trivial k_π^{n-1} components and G denote the corresponding overlap graph.*

If $(V_1, V_2) \in G$ and $\xi : \mathcal{N}_h \rightarrow \mathbb{R}$ then there exists a unique $c \in \mathbb{R}$ at which

$$g(c) = \sum_{i \in V_1 \cap V_2} \gamma^*(\xi_i + c) - s_{1i}^{n-1}(\xi_i + c)$$

is minimal.

Proof. Under Assumptions 3.1 g is continuously differentiable with

$$\lim_{c \rightarrow -\infty} g'(c) = - \sum_{i \in V_1 \cap V_2} s_{1i}^{n-1} < 0 \quad \text{and} \quad \lim_{c \rightarrow \infty} g'(c) = - \sum_{i \in V_1 \cap V_2} 1 - s_{0i} - s_{1i}^{n-1} = \sum_{i \in V_1 \cap V_2} s_{2i}^{n-1} > 0.$$

The strict inequalities follow since $k_\pi(0) = 0$ and the lemma guarantees there are nodes where $0 \neq k_\pi^{n-1} = k_\pi(s_\pi^{n-1})$ for $\pi = 1$ and 2. The intermediate value theorem and convexity of

g guarantee the existence of an interval $[c_1, c_2]$ upon which g takes its minimal value and g' vanishes.

To establish uniqueness it suffices to show that at a minimum there exists $i \in V_1 \cap V_2$ for which $\xi_i + c < \hat{\xi}_i$ since $\gamma^*(\xi_i + c)$ is strictly convex on $(-\infty, \hat{\xi}_i)$. This is immediate; if $\xi_i + c \geq \hat{\xi}_i$ at every node, then

$$g'(c) = \sum_{i \in V_1 \cap V_2} 1 - s_{0i} - s_{1i}^{n-1} = \sum_{i \in V_1 \cap V_2} s_{2i}^{n-1} > 0,$$

contradicting $g'(c) = 0$. \square

3.4. Fully Degenerate Case. In the absence of additional assumptions on the permittivities and surface tension, uniqueness of minimizers of $\tilde{\Psi}_h$ can be established when the domain Ω satisfies the geometric hypotheses in the following theorem.

THEOREM 3.6. *Let $\Omega \subset \mathbb{R}^d$ be a connected domain with $\mathbb{R}^d \setminus \Omega$ connected, and let \mathcal{T}_h be a simplicial triangulation of Ω with node set \mathcal{N}_h . If $k_\pi : \mathcal{N}_h \rightarrow [0, \infty)$ satisfy $k_1(v) + k_2(v) > 0$ then the corresponding overlap graph is a tree.*

The proof of this theorem is presented in the appendix.

THEOREM 3.7. *Let $\Omega \subset \mathbb{R}^d$ be a connected domain with $\mathbb{R}^d \setminus \Omega$ connected, and let \mathcal{T}_h be a Delaunay triangulation of Ω with node set \mathcal{N}_h . If the permittivities k_π , interfacial energy γ , and triangulation satisfy Assumptions 3.1, then minima of the function $\tilde{\Psi}_h : \mathbb{R}^{|\mathcal{N}_h|} \times \mathbb{R}^{|\mathcal{N}_h|} \rightarrow \mathbb{R}$ in equation (3.2) are unique.*

Proof. Define $k_\pi^{n-1} : \mathcal{N}_h \rightarrow \mathbb{R}$ to be the functions with values $k_{\pi i}^{n-1} = k_\pi(s_{\pi i}^{n-1})$, and let \mathcal{V}_π denote the set of non-trivial k_π^{n-1} components and G denote the corresponding overlap graph characterized in Definition 3.3.

Let \mathbf{p} and $\tilde{\mathbf{p}}$ be two minima of $\tilde{\Psi}$ and write $\xi_i = p_{1i} - p_{2i}$ and $\tilde{\xi}_i = p_{t1i} - \tilde{p}_{2i}$. The hypothesis on γ^* and k_π imply $k_{\pi ij}^{n-1} > 0$ for every edge (i, j) of \mathcal{T}_h with nodes $i, j \in V_\pi \in \mathcal{V}_\pi$. Since nodes in the components V_π are connected by edges in \mathcal{T}_h it follows from equation (3.3) that:

- The differences $p_{\pi i} - \tilde{p}_{\pi i}$ are constant on components $V_\pi \in \mathcal{V}_\pi$ for $\pi = 1$ and 2 .
- $\xi_i = \tilde{\xi}_i$ on the degenerate set $\mathcal{N}_{0h}^{n-1} = \mathcal{N}_{1h}^{n-1} \cup \mathcal{N}_{2h}^{n-1}$. This follows since $k_{\pi ij}^{n-1} = 0$ if $i \in \mathcal{N}_{\pi h}^{n-1}$ in which case $p_{\pi i}$ and $\tilde{p}_{\pi i}$ are free to minimize $\xi \mapsto \gamma^*(\xi) - s_1^{n-1}\xi + \max(0, \xi - \hat{\xi}_i)^2$ which is strictly convex.

Note too that if $i \in \mathcal{N}_{\pi h}^{n-1}$ then $k_{\pi i}^{n-1} = 0$, and since $k_{1i}^{n-1} + k_{2i}^{n-1} > 0$ that $i \in V_{\pi'} \in \mathcal{V}_{\pi'}$ where $\pi' = 1$ if $\pi = 2$ and visa versa. Thus if $p_{\pi' i} = \tilde{p}_{\pi' i}$ on $V_{\pi'}$ then $\xi_i = \tilde{\xi}_i$ implies $p_{\pi i} = \tilde{p}_{\pi i}$; that is, uniqueness on the non-degenerate components implies uniqueness on the degenerate set.

We show that the differences $p_{\pi i} - \tilde{p}_{\pi i}$ take the same constant c on every component $V_\pi \in \mathcal{V}_\pi$ for $\pi = 1$ and 2 . Uniqueness then follows since the averages of $p_1 + p_2$ and $\tilde{p}_1 + \tilde{p}_2$ vanish;

$$0 = \sum_{i \in \mathcal{N}_i} |C_i| ((p_{1i} + p_{2i}) - (\tilde{p}_{1i} + \tilde{p}_{2i})) = 2 \sum_{i \in \mathcal{N}_i} |C_i| c = 2|\Omega|c.$$

Since the overlap graph is connected, it suffices to show that for each pair of components $(V_1, V_2) \in G$ the constant value of $p_{1i} - \tilde{p}_{1i}$ on V_1 is equal to the constant value of $p_{2i} - \tilde{p}_{2i}$ on V_2 .

Fix $(V_1, V_2) \in G$ and write $p_{\pi i} - \tilde{p}_{\pi i} = c_\pi$ for the constant values the differences take on V_π . Then

$$\xi_i - \tilde{\xi}_i = (p_{1i} - p_{2i}) - (\tilde{p}_{1i} - \tilde{p}_{2i}) = c_1 - c_2 \equiv \delta, \quad i \in V_1 \cap V_2.$$

To show that $\delta = 0$ we verify that the function

$$g(c; \xi) = \sum_{i \in V_1 \cap V_2} \gamma^*(\xi_i + c) - s_{1i}^{n-1}(\xi_i + c)$$

is minimized when $c = 0$ and similarly $g(c; \tilde{\xi})$ is minimized when $c = 0$. Since $\xi = \tilde{\xi} + \delta$ on $V_1 \cap V_2$ we find

$$g(c; \xi) = g(c; \tilde{\xi} + \delta) = g(c + \delta; \tilde{\xi}),$$

and the strict convexity of $g(c; \xi)$ at the minimum established in Corollary 3.5 implies $\delta = 0$.

To show that $g(c; \xi)$ is minimized when $c = 0$ we use the property that G is a tree and \mathbf{p} minimizes $\tilde{\Psi}_h(\mathbf{p})$. Since G is a tree, deleting the edge (V_1, V_2) gives two disconnected sub-trees, $G \setminus (V_1, V_2) = G_L \cup G_R$ and the subsets of \mathcal{N}_h given by

$$\mathcal{N}_L = \bigcup_{(U_1, U_2) \in G_L} U_1 \cup U_2 \quad \text{and} \quad \mathcal{N}_R = \bigcup_{(U_1, U_2) \in G_R} U_1 \cup U_2,$$

have intersection $\mathcal{N}_L \cap \mathcal{N}_R = V_1 \cap V_2$. Define $\mathbf{q} : \mathcal{N}_h \rightarrow \mathbb{R}^2$ by $\mathbf{q}_i = (p_{1i} + c, p_{2i} + c)$ if $i \in \mathcal{N}_R$ and $\mathbf{q}_i = \mathbf{p}_i$ otherwise. Since shifting \mathbf{q} by a constant (\bar{q}, \bar{q}) so that $q_1 + q_2$ averages to zero does not alter $\tilde{\Psi}_h(\mathbf{q})$, and since \mathbf{p} minimizes $\tilde{\Psi}$, it follows that

$$0 \leq \tilde{\Psi}_h(\mathbf{q}) - \tilde{\Psi}_h(\mathbf{p}) = g(c; \xi) - g(0; \xi), \quad c \in \mathbb{R};$$

that is, $c \mapsto g(c; \xi)$ is minimized at $c = 0$. Similarly, since $\tilde{\mathbf{p}}$ also minimizes $\tilde{\Psi}_h$ it follows that $c \mapsto g(c; \tilde{\xi})$ is also minimized at $c = 0$. \square

3.5. Partially Degenerate Case. The conjugate of the interfacial energy illustrated in Figure 2.2 is non-negative so that $s_1 = (\gamma^*)'(p_1 - p_2) > 0$ is always non-negative. If $k_1(s_1)$ only vanishes when $s_1 = 0$, then $k_{1ij}^{n-1} > 0$ for all edges (n_i, n_j) of \mathcal{T}_h so that \mathcal{V}_1 consists of a single component. In this situation the overlap graph G is a star so is trivially a tree. The requirement that $\mathbb{R}^d \setminus \Omega$ be connected can then be omitted from the hypothesis of Theorem 3.7.

THEOREM 3.8. *Let $\Omega \subset \mathbb{R}^d$ be a connected domain and let \mathcal{T}_h be a Delaunay triangulation of Ω with node set \mathcal{N}_h . Let the permeabilities k_π , interfacial energy γ , and triangulation satisfy Assumptions 3.1 and assume that $k_1(s) = 0$ if and only if $s = 0$. Then minima of the function $\tilde{\Psi}_h : \mathbb{R}^{|\mathcal{N}_h|} \times \mathbb{R}^{|\mathcal{N}_h|} \rightarrow \mathbb{R}$ specified in equation (3.2) are unique.*

The assumption on k_1 may be relaxed if, for example, a maximum principle is available [14] to establish s_1 is bounded below by a constant $\hat{s}_1 > 0$ for which $k_1(s) > 0$ when $s \in (\hat{s}_1, 1]$.

4. Well Models and Non-Homogeneous Equations. Naive inclusion of non-homogeneous terms on the right hand side of equation (2.1) gives rise to a term of the form $\mathbf{q} \cdot \mathbf{p}$ in equation (2.5) for $\Psi(\mathbf{p})$. Since Ψ only has linear growth this can lead to a loss of existence and uniqueness of minimizers⁴. In order to model the pressures and fluxes in wells (holes) where fluid may

⁴The prototypical example is $\Psi(p) = |p| - qp$ for $p \in \mathbb{R}$. If $|q| < 1$ minimizers exist and are unique, if $|q| = 1$ minimizers exist but are not unique, and when $|q| > 1$ there are no minimizers.

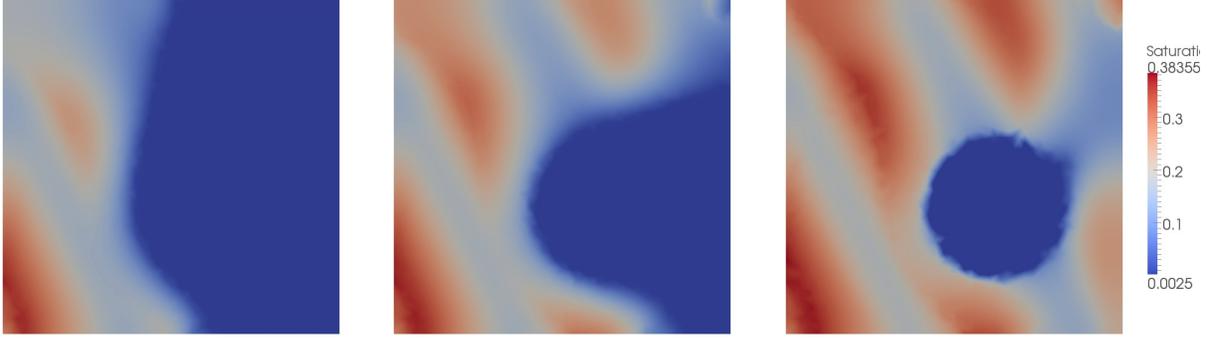


FIG. 5.1. Saturations of injected fluid at times $t = 1, 1.75, 5$.

enter and exit it is common to include a term of the form $W(\mathbf{p}_0 - \mathbf{p})$ at well locations to the right hand side of equation (2.1) [7, Chapter 13]. Here $W \in \mathbb{R}^{d \times d}$ is symmetric and positive definite and the “bottom hole pressure” \mathbf{p}_0 is specified. This gives an additional term of the form $Q(\mathbf{p}) = (1/2)|\mathbf{p} - \mathbf{p}_0|_W^2$ on the right equation (2.5) for $\Psi(\mathbf{p})$. Since this term is non-negative $\Psi + Q$ is coercive whenever Ψ is, so the existence of solutions follows mutatis mutandis as in Theorem 3.2. However, proofs of uniqueness exploited the invariance of Ψ under translations of the form $(p_1, p_2) \mapsto (p_1 + c, p_2 + c)$ which typically will not hold for $\Psi + Q$.

5. Numerical Example. A numerical example with prototypical fluid and medium properties and significant degeneracy is presented to illustrate the robustness of the formulation. Nondimensionalizing equations (2.1) with characteristic time $T = 10^7 s$ (a year), length $L = 10^3 m$ (kilometers), and pressure $P = 10^6 Pa$, gives non-dimensional equations of the same form with the permeability scaled by $TP/L^2 = 10^7$. For prototypical geological problems [9] the permeability of the medium is $K = O(10^{-10})m^2$ and fluid viscosities $\mu = O(10^{-3})Pa s$, so the permeability $k \simeq K/\mu$ for the non-dimensional equations is of order $O(1)$. With this scaling all computed quantities are well centered in the floating point range. The following parameters were selected to model layered medium in a two kilometer square domain, $\Omega = [-1, 1]^2$, with an impermeable depression of radius $\ln(1.25)/2 \simeq 0.11$ centered at $c = (1/4, -1/4)$. An injection well is located in the lower left corner $(-1, 1)$ and production at the upper right corner $(1, 1)$.

- Domain: $[-1, 1]^2$ with $0 \leq t \leq T = 5$.
- Boundary Data: No flux for each fluid.
- Volume ratio of medium: $s_0(x) = 0.7 + 0.1 \sin(2x_1 + x_2)$, porosity $\phi = 1 - s_0$.
- Medium Permeability: $K_0/\mu = 2.5 \max(\exp(|x - c|^2) - 1.25, 0)I$ with $c = (1/4, -1/4)$ and the viscosities for each fluid were taken to be the same, $\mu = \mu_1 = \mu_2$.
- Phase Permiabilities: $K_\pi(s_\pi) = s_\pi \max(0, s_\pi - 0.1(1 - s_0))K_0$.
- Wells: $Q(x, \mathbf{p}) = (1/2)(p_1 - 60)^2 \chi_{B_{1/8}(-1, -1)}(x) + (1/2)|\mathbf{p}|^2 \chi_{B_{1/8}(1, 1)}(x)$.
- Interfacial Energy: With $p^* \equiv -1/(2\sqrt{1 - s_0})$ and $s_0 = s_0(x)$ as above,

$$\gamma^*(p_1 - p_2) = \begin{cases} (1 - s_0)(p_1 - p_2) & p_1 - p_2 \leq p^* \\ -1/(4(p_1 - p_2)) - \sqrt{1 - s_0} & \text{otherwise} \end{cases}$$

This is the conjugate function from Example 2.2.

- Initial Data: $\mathbf{s} = \partial(I_L + \Gamma)^*(\mathbf{p})$ with $\mathbf{p} = (-5, 5)$ is computed with equation (2.2).

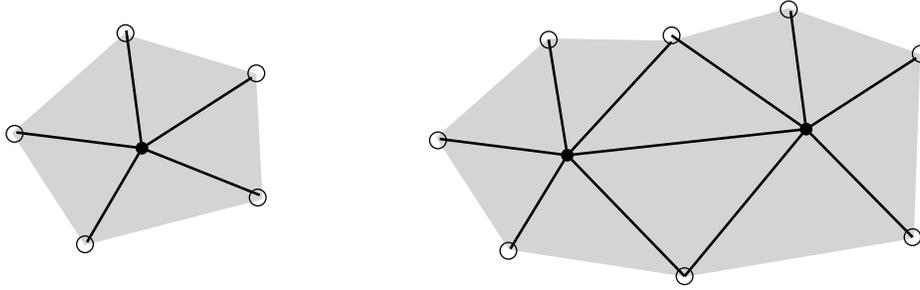


FIG. A.1. Proof of Lemma A.3: neighborhood of $n \in A$ (left) and two adjacent points in A (right).

Figure 5.1 illustrates the saturation of the injected fluid obtained with this data at three times:

- Left: the injected fluid is forced towards the top around the impervious region.
- Middle: The injected fluid reaches the production well (breakout). The layered medium has porosity in the range $0.2 \leq 1 - s_0 \leq 0.4$ and the injected fluid has saturated the pores in the lower left portion of the domain.
- Right: At the final time the injection fluid has surrounded the impenetrable region and is slowly displacing residual amounts of the second fluid from the narrow region on the right. The injected fluid forms the majority of fluid emanating from the production well.

This solution was computed using 512 time steps ($\tau = 5/512$) on a Delaunay mesh [22] with 1592 vertices (two pressures per vertex), and 3061 triangles. The solution at each step was computed as a minima of the convex function $\tilde{\Phi}_h$ given in equation (3.2) using 50 Nesterov iterations to obtain an initial approximation for the semi-smooth Newton scheme of Figure 2.3 which, for this example, then converged in 3-5 iterations.

Appendix A. Proof of Theorem 3.6.

The proof of the tree property of overlap graphs utilizes multiple notions of connectedness.

NOTATION A.1. *Triangulations of a domain will be denoted by \mathcal{T} and the node set by \mathcal{N} . We write $K \in \mathcal{T}$ if K is a simplex (node, edge, ...) of \mathcal{T} .*

- $A \subset \mathbb{R}^d$ is connected if it can not be covered by two disjoint open sets. Open sets in \mathbb{R}^d are locally path connected, so if A is open it is connected if and only if it is path connected.
- $A \subset \mathcal{N}$ is edge connected (in \mathcal{T}) if for any two nodes in A there is a path from one to the other in the edge set of \mathcal{T} with vertices in A .
- Given functions $k_\pi : \mathcal{N} \rightarrow \mathbb{R}$, the notion of k_π connectedness of Definition 3.3 is utilized. Note that if $A \subset \mathcal{N}$ is k_π connected then it is edge connected.

These are all equivalence relations so give rise to disjoint partitions into (maximally)⁵ connected components.

The proof of Theorem 3.6 uses the following simple but subtle theorem from algebraic topology [10].

THEOREM A.2. *Let $A \subset \mathbb{R}^d$ be open and connected. The complement $A^c = \mathbb{R}^d \setminus A$ is connected if and only if the boundary ∂A of A is connected.*

⁵The maximal property of components follows from their definition as equivalence classes. The redundant use of *maximal* is used when it is the essential property for an argument.

The following lemma is a discrete analog of the non-trivial implication of this theorem. In this lemma the distance $d(m, n)$ between nodes in \mathcal{N} is the least number of edges in a path in the edge set of \mathcal{T} connecting them.

LEMMA A.3. *Let \mathcal{T} be a simplicial triangulation of \mathbb{R}^d with node set \mathcal{N} , and let $d(m, n) \in \mathbb{N}$ denote the distance between nodes in the edge set of \mathcal{T} . If $\mathcal{A} \subset \mathcal{N}$ is an edge connected set of nodes and the complement $\mathcal{A}^c = \mathcal{N} \setminus \mathcal{A}$ is also edge connected, then the set of nodes $d_1(\mathcal{A}) \equiv \{n \in \mathcal{N} \mid d(n, \mathcal{A}) = 1\}$ is edge connected. That is, if $m, n \in d_1(\mathcal{A})$ then there is a path of edges in \mathcal{T} from m to n with nodes in $d_1(\mathcal{A})$.*

Proof. In order to use Theorem A.2 we define the open set (see Figure A.1)

$$A = \mathcal{A} \cup \bigcup_{n \in \mathcal{A}} \{\overset{\circ}{K} \mid n \in K, K \text{ a simplex in } \mathcal{T}\} \subset \mathbb{R}^d.$$

Here $\overset{\circ}{K}$ denotes the interior of a simplex (edge, triangle, tetrahedron) K . To show that A and $A^c \equiv \mathbb{R}^d \setminus A$ are connected we use the property that $\mathcal{N} \cup_{K \in \mathcal{T}} \overset{\circ}{K}$ is a disjoint partition of \mathbb{R}^d . Then,

- If (m, n) is an edge in \mathcal{T} with $m, n \in \mathcal{A}$, then the segment $[m, n] \subset A$ by construction. Conversely, if $m, n \in \mathcal{A}^c$ then the open segment $(m, n) \not\subset A$, so $[m, n] \subset A^c$. By hypothesis \mathcal{A} is edge connected so any two vertices in \mathcal{A} are connected by a path in A , and similarly two nodes in \mathcal{A}^c are connected by a path in A^c .
- Every point $x \in \mathbb{R}^d \setminus \mathcal{N}$ is in the interior of a simplex $K \in \mathcal{T}$. If K contains a node in \mathcal{A} then $x \in \overset{\circ}{K} \subset A$; otherwise, $x \in K \subset A^c$. Since $\overset{\circ}{K}$ is convex there is a path $[x, n] \subset \overset{\circ}{K}$ from x to any node $n \in \partial K$.
- It follows that any two points $x, y \in A$ (resp. A^c) can be connected by a path of the form $[x, m] \cup [m, n] \cup (n, y] \subset A$ (resp. $\subset A^c$), with m and n nodes of \mathcal{A} (resp. \mathcal{A}^c).

Theorem A.2 then shows that the (topological) boundary ∂A of A is connected. We next show that $\mathcal{N} \cap \partial A = \{n \in \mathcal{T} \mid d(n, \mathcal{A}) = 1\}$.

Superset: $\mathcal{N} \cap \partial A \supset d_1(\mathcal{A})$. If $d(n, \mathcal{A}) = 1$ then there exists an edge $[m, n]$ of \mathcal{T} with $m \in \mathcal{A}$. Then $[m, n) \subset A$ so $n \in \partial A$.

Containment: $\mathcal{N} \cap \partial A \subset d_1(\mathcal{A})$. Since A is open it follows that $A \cap \partial A = \emptyset$ so it is immediate that $d(n, \mathcal{A}) > 0$ when $n \in \mathcal{N} \cap \partial A$; we show $d(n, \mathcal{A}) < 2$.

Let $n \in \mathcal{N}$ with $d(n, \mathcal{A}) \geq 2$ and let K be a simplex containing it; $n \in K \in \mathcal{T}$. Since $d(m, n) = 1$ for every node $m \in K$ it follows from the triangle inequality that $m \notin \mathcal{A}$ so $\overset{\circ}{K} \not\subset A$. Then

$$\{n\} \cup \{\overset{\circ}{K} \mid n \in K, K \text{ a simplex in } \mathcal{T}\} \subset A^c$$

is an open neighborhood of n disjoint from A ; in particular, $n \notin \partial A$.

To conclude that $d_1(\mathcal{A})$ is edge connected it suffices to show $\{K \subset \partial A \mid K \in \mathcal{T}\}$ is a triangulation of ∂A . If $x \in \partial A \setminus \mathcal{N}$, let $K \in \mathcal{T}$ be the (unique) simplex for which $x \in \overset{\circ}{K}$.

- K does not have a node in \mathcal{A} since otherwise $x \in \overset{\circ}{K} \subset A$.
- Since $x \in \partial A$ every neighborhood of x intersects A ; in particular, $x \in \partial K'$ for some d simplex with $\overset{\circ}{K}' \subset A$. (If $\overset{\circ}{k} \subset A$ and $k \subset K'$ then $\overset{\circ}{K}' \subset A$.) Since \mathcal{T} is a triangulation it follows that $K \subset K'$ (a d simplex contains any sub-simplex that it intersects).

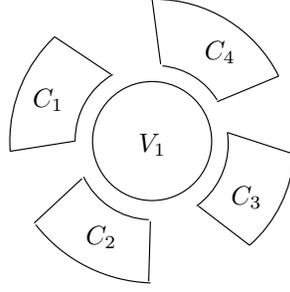


FIG. A.2. Partition of node set \mathcal{N} in the proof of Theorem A.4.

- It follows that $K \subset \bar{A}$ and does not contain a vertex of \mathcal{A} so $K \not\subset A$ whence $K \subset \bar{A} \setminus A = \partial A$.

□

We first prove the tree property when $\Omega = \mathbb{R}^d$; the proof of Theorem 3.6 will then be deduced from this.

THEOREM A.4. *Let \mathcal{T}_h be a simplicial triangulation of \mathbb{R}^d with node set \mathcal{N}_h . If $k_\pi : \mathcal{N}_h \rightarrow [0, \infty)$ satisfy $k_1(v) + k_2(v) > 0$ then the corresponding overlap graph is a tree.*

Proof. Suppose to the contrary that G contains a cycle. Then there exist vertices $V_1, \tilde{V}_1 \in \mathcal{V}_1$ of G and paths P and \tilde{P} from V_1 to \tilde{V}_1 in G for which the end points are the only vertices in common. We establish a contradiction by showing that there is a vertex $V_2 \in \mathcal{V}_2$ of G common to both paths.

Let C_1, C_2, \dots, C_M be the edge connected components of $\mathcal{N} \setminus V_1$. Then $V_1 \cap \tilde{V}_1 = \emptyset$ so $\tilde{V}_1 \subset \mathcal{N} \setminus V_1$ and \tilde{V}_1 is edge connected, so without loss of generality assume $\tilde{V}_1 \subset C_1$. Since the components are pairwise disjoint it follows that

$$C_1^c \equiv \mathcal{N} \setminus C_1 = V_1 \cup \bigcup_{i=2}^M C_i;$$

moreover, this is a disjoint partition (see Figure A.2).

Claim: C_1^c is an edge connected subset of \mathcal{N} .

Proof: For any two nodes $n \in V_1$ and $m \in C_i$ there exists a path p in the edge set of \mathcal{T} joining them. Since the C_i are (maximally) edge connected components there are no edges between any two of them, thus the sub-path p' of p starting with the last edge to enter C_i is a path from some $n' \in V_1$ to m and is contained in $V_1 \cup C_i$. Since V_1 is edge connected it follows there is a path q from n to n' in V_1 . Then $q + p'$ is a path from n to m in $V_1 \cup C_i$, and since $i \geq 2$ is arbitrary the claim follows. *QED*

Then C_1 and C_1^c are edge connected subsets of \mathcal{N} , it follows from the previous lemma that $d_1(C_1^c) \equiv \{n \in \mathcal{N} \mid d(n, C_1^c) = 1\}$ is edge connected.

Claim: $d_1(C_1^c) \subset d_1(V_1)$.

Proof If $d(n, C_1^c) = 1$ there exists an edge (m, n) in \mathcal{T} for which $n \in C_1$ and $m \in C_1^c$. Since $\{C_i\}$ are (maximally) connected edge components there are no edges between them, in particular, $d(m, n) > 1$ for any $m \in \bigcup_{i=2}^M C_i$. It follows that $m \in V_1$. *QED*

To complete the proof, suppose V_1 and $\tilde{V}_1 \in \mathcal{V}_1$ are distinct vertices of G and there exist paths P and P' in the edge set of G connecting them which intersect only at the end points. Since k_π components are edge connected in \mathcal{T} , it follows from the definition of the overlap graph that for any $m \in V_1$ and $n \in \tilde{V}_1$ there exist paths p and p' in the edge set of \mathcal{T} from m to n which only intersect in V_1 and \tilde{V}_1 .

Since $V_1 \subset C_1^c$ and $\tilde{V}_1 \subset C_1$, each path p and p' must exit C_1 ; in particular, there are edges (m, n) and (m', n') on these paths for which $m, m' \in C_1$ and $n, n' \notin C_1$ so that $d(n, C_1) = d(n', C_1) = 1$.

Since V_1 is a (maximally) k_1 -connected component it follows that $k_1(i) = 0$ for any vertex for which $d_1(i, V_1) = 1$, hence $k_2(i) > 0$. In particular, $k_2(i) > 0$ for every vertex $i \in d_1(C_1)$ and $d_1(C_1)$ is also edge connected, so $d_1(C_1) \subset V_2$ for some k_2 component $V_2 \in \mathcal{V}_2$.

The contradiction now follows since $n \in V_2$ and $n' \in V_2$ shows V_2 is a vertex of G on each path from V_1 to \tilde{V}_1 . \square

Proof. (of Theorem 3.6) Let \mathcal{T} be a triangulation of a connected domain $\Omega \subset \mathbb{R}^d$ and $k_\pi \rightarrow [0, \infty)$ satisfy $k_1(n) + k_2(n) > 0$ at every node of \mathcal{T} , let and G denote the corresponding overlap graph. Extending \mathcal{T} to a triangulation \mathcal{T}' of \mathbb{R}^d setting $k_\pi(n) = 1/2$ for nodes n not in \mathcal{T} gives a triangulation and functions satisfying the hypothesis of the previous theorem so that the overlap graph G' for the extended triangulation and functions is a tree. Since k_π components of \mathcal{N} are contained in k_π -components of \mathcal{N}' it follows G is a sub-graph of G' , so is a forest. However, Lemma 3.4 shows G is connected, so it is a tree. \square

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