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TECHNICAL WHITEPAPER

A Priori identification of the instantaneous spatiotemporal support of change

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Abstract

Petroleum recovery processes invariably couple physical phenomena that are characterized by a disparate range of spatiotemporal scales. While flow state variables evolve on a global scale, reactive transport waves travel with a distinctly local support. This whitepaper outlines a research program that seeks to characterize the spatiotemporal evolution of the multiscale flow and transport systems that are central to petroleum recovery processes broadly. It is hypothesized that the nonzero spatial support of the instantaneous change in state variables can be predicted. Moreover, it is conjectured that certain closed form analytical models that depend solely on known parameters of the system provide *a priori* characterizations of the support.

The proposed work adopts an analytical approach. The approach first proceeds by forming the fully-implicit, semidiscrete in time, set of equations. This is followed by the application of an infinite-dimensional Newton process in order to obtain the updated state. In this process, each iterate is the solution of a linear, steady Partial Differential Equation; the solution itself is the Newton Update that generates the iterates. The sum of the update functions is the instantaneous change in state over the timestep. Through obtaining these updates, it is conjectured that the spatial support of the nonzero changes can be determined analytically. Through the accuracy of fully-discrete approximations, the results on the continuous domain are extended to the discrete problem.

It is anticipated that general nonlinear and heterogenous flow components evolve according to a linear screened Poisson equation, transport terms evolve as first order initial value problems.

The practical implications of this work are far-reaching; uncertainty quantification and simulation model developers will know the precise locality of any dynamic multiphase displacement before knowing its complete state. This can lead to the development of numerical techniques in multiscale numerical simulation of oil and gas recovery that perform on orders of magnitude more computationally efficiently.

Contents

1 Introduction

Petroleum recovery processes invariably couple physical phenomena that are characterized by a disparate range of spatiotemporal scales [6, 30]. A first-order source of such coupling is within the constitutive relations for flow in porous media that arise through the volume averaging process of continuum modeling. One specific example of this is the coupling between pressure and saturation *via* the multiphase extension to Darcy's law [34]. Physical systems that involve such character are referred to as *multiscale* systems. Another source of coupling across scales arises in petroleum recovery processes due to the fact that the overall integrated process will often involve multiple types of Physics. For example, geomechanics and multiphase flow are coupled to well-bore flow [37]. Such systems are referred to as *multiphysics* systems. The proposed work seeks to further our understanding of the spatiotemporal evolution of multiscale and multiphysics systems that are central to petroleum recovery systems broadly. The proposed approach is analytical, and it is restricted to the focal setting of petroleum recovery systems that are modeled by a certain canonical form. This canonical form is introduced mathematically later in this section. The canonical form encompasses the general governing equations for transient multiphase multicomponent flows in heterogeneous porous media with the possibility for chemical reactions and coupling to advanced well-bore flows.

Multiscale and multiphysics coupling is invariably accompanied by an inherent, and dynamically evolving, spatiotemporal locality. While one set of Physics evolves globally, other phenomena exhibit a relatively local evolution. There is further complexity in such physical systems; the transitions across characteristic regimes, and the scale separations across various coupled subprocesses are often nonlinear and state dependent. Subsequently, the precise nature of the spatiotemporal locality in the evolution of state variables is difficult to characterise. In general heterogeneous and nonlinear settings, analytical models of such systems are limited, and Numerical Simulation is necessary for the purposes of modeling for prediction and assessment [4, 12].

The numerical simulation of multiscale and multiphysics systems is fundamentally challenged

by a curse of dimensionality. Specifically, in numerical simulation, the space-time domain is discretized and approximations of the state variables at discrete points or elements are sought. The *resolution* of the discrete domain refers to level of granularity of the discretization, whereas the *extent* of the domain refers to its overall size. The dimensionality of the discrete domain is the product of the resolution and the extent. In multiscale and multiphysics systems, the global Physics will dictate the extent of the discrete spatial and temporal domain while the local Physics will dictate its resolution. The wider the gap between the global and local characteristic scales, the larger the dimensionality of the full-resolution discrete system. Both globally and locally evolving state variables need to be solved under the same imposed dimension of the discrete domain. This implies that the computational complexity of such simulations is far greater than the intensity of change in the physical variables.

This leads to a timely topic of research in the design of numerical simulation methods. Modern advances in the simulation of such phenomena aim to take advantage of the spatiotemporal locality of the evolution of certain state variables in order to reduce the necessary computational effort [21]. Ideally, and especially in light of the geometric growth in the complexity of emerging applications, this is accomplished with an amount of computation that is directly proportional to the amount of change in state variables.

Next we review methods in Numerical Simulation that strive to exploit locality in one form or another. These methods form the potential areas of research that can benefit from the proposed work in this whitepaper.

1.1 Review of methods that exploit spatiotemporal locality

Modern simulation methods for complex nonlinear multiscale problems overwhelmingly follow the Adaptive Discretization paradigm. In this paradigm, the numerical approximation itself is adaptively modified in space, time, or both in order to improve the method's computational efficiency. In doing so, while the objective of adaptive computation is often achieved, the integrity of

the approximations' accuracy and robustness may be compromised or require additional effort for it to be maintained.

One example of a promising Adaptive Discretization method is Adaptive Mesh Refinement or Dynamic Gridding [9, 22, 41, 20]. In these methods, the spatial discretization of the domain is dynamically altered by refining its resolution in locales where changes in state are occurring locally and by coarsening the resolution otherwise. This class of method is particularly effective for homogeneous problems that evolve with a predominant travelling-wave character. Under heterogeneity, homogenization strategies are necessary every time the mesh is adapted [20]. This leads to additional computational expense, and more importantly, to additional approximation errors associated with the homogenization process. For problems that have components which evolve with a more global character, the efficacy of Adaptive Mesh Refinement methods is relatively limited. Advances in the identification of locality can help mitigate some of the concerns surrounding the use of AMR.

Another promising Adaptive Discretization method is the use of a spatially varying temporal discretization [19, 17]. These methods are also referred to as local time-stepping or adaptive time-step refinement methods [32, 35]. In this class of method, parts of the domain where a state variable is experiencing rapid change, the numerical integration is performed using a fine temporal resolution compared to other locales. While such methods are proving to be effective for hyperbolic problems that involve sharp frontal advancement, there are potentially serious challenges to their application for parabolic problems with more global character. In particular, for such problems, synchronization strategies are required in order to inform neighboring locales of the locally occurring rapid changes in state. Reliable *a priori* knowledge of any locality that may be present could lead to a class of local timestepping methods that are effective even for parabolic problems. In such schemes, there would be no need for any synchronization despite the parabolic character.

Adaptive Multiscale methods are an alternate form of Adaptive Discretization strategy that do not rely on the dynamic adaptation of the discrete domain [1, 25, 26, 33]. Rather, in this

approach, the state variables that evolve on a more global scale are integrated using coarsened representations. These representations are tied to the remaining state variables that are represented by fine scale equations.

An emerging alternate paradigm to the Adaptive Discretization class of method is the Adaptive Solver approach. In the Adaptive Solver approach, the key idea is to apply full-resolution, fully-coupled approximations that are static, and to innovate underlying solvers that are themselves dynamically adaptive to a varying spatiotemporal support. Since the numerical approximation itself is unmodified, there are no impending fidelity or accuracy concerns and these methods can in principle combine the efficiency of adaptive computation with the fidelity of well-established numerical approximations. Examples in this class of method include adaptive localization strategies [47] and solutions that exploit potential based orderings [29]. Another example is the development of adaptive nonlinear preconditioners that are based on domain decomposition ideas [11, 24]. These nonlinear solvers were recently applied to basic petroleum recovery applications [39, 38].

All of these adaptive numerical methods require the answer to one fundamental question in one form or the other. Given a particular instant in time, suppose that we are informed of the present dynamic and static states of the system that is under study. In what part of the spatial domain will the dynamic state experience change? This part of the domain is called the *support* as it supports nontrivial instantaneous changes in state. What does the support depend on and how?

1.2 Associated work on the topic of locality

The character of the evolution of flow and transport state variables and of their associated spatial supports is complex. Moreover, as discussed in the previous section, an accurate characterisation of this evolution is paramount for the future success and efficiency of simulation methods for emerging multiscale and multiphysics petroleum recovery processes. In the broadest context, the spatiotemporal locality of dynamic change continues to be a subject of study [23], and in the more specific context of general multiphase flow and transport, there is still no fundamental and

universally applicable characterization of it. In this section, we first review associated work on the topic. This is followed by a technical introduction to the proposed approach towards a fundamental and universally applicable characterization.

In the literature, there are two approaches to the study of locality and to the development of ways to exploit it in computation. The first approach is **indirect** and seeks to characterize locality through the study of the resulting approximation errors in models for the system. Classic examples of such work include the error estimate derivations [5, 44] and the reviews [2, 42], as well as several recent applications such as [36, 48, 15, 40]. These and other successful error-based adaptivity investigations and applications are well-established for the flow (Equation 2.2), transport (Equation 2.3), and coupled (Equation 2.1) problems.

The second approach towards characterizing and exploiting locality that is reported on in the literature is **direct**. Direct studies of locality in unrelated physical systems include the flow of traffic [43], which exhibits a travelling wave character, and accretive transport phenomena [31]. On the other hand, in studies that are focused on flow and transport phenomena, works following the direct approach are further categorized as either (a) those that tackle general systems while seeking to devise *ad hoc* characterisations, or (b) those that deal with limiting cases and idealized systems while seeking exact and analytical results. Examples of the former, are the sharp discontinuity detection procedures that are applicable to transport problems [8, 7, 10]. In these procedures, the focus is on the detection of fronts and in the application of linearized approximations and local Courant-Friedrichs-Lewy numbers to guess the support. Examples of the latter are studies regarding the notion of a *radius of investigation* in pressure transients about wells in flow problems [28, 45, 14]. In these studies, while idealizations are made regarding the limitation on the phases present and on the level and nature of the underlying homogeneity, the results are exact.

The motivation for the present proposed work stems from a recent advance that was made at FuRSST [46]. In this advance, a direct approach is taken to the study of locality in decoupled flow and transport systems. The approach tackles general flow and transport problems that incorporate

general nonlinearity and heterogeneity in one-dimension. The study derives a sharp analytical bound that characterizes the spatiotemporal support of change for decoupled flow and transport systems. It achieves this by utilizing the infinite-dimensional Newton method [16], and it provides links to the discrete problem through recent developments in the derivation of an Asymptotic Mesh Independence Principle [3, 27].

The proposed work will focus on a specific and yet broad setting for multiphase flow and transport. For this setting, a hypothesis regarding the character of the instantaneous spatiotemporal support is made. The proposed work makes conjectures of specific estimates for the size, location, and rate of growth of the support that depend on parameters that are already known. It is then proposed that an innovative analytical framework be applied in order to validate and analyze the hypothesised conjectures.

2 Canonical problem and formal objectives

The physical system that that the proposed work focuses on concerns the evolution of two sets of independent state variables. The first set groups state variables that evolve under a more global support. These variables are called *flow variables*, and are denoted as $p(\mathbf{x}, t)$, where $\mathbf{x} \in \mathbb{R}^3$ is a position vector, and $t \geq 0$ is time. The second collection of variables evolves with a relatively local character. They are called *transport variables* and are denoted as $s(\mathbf{x}, t)$. The flow and transport state variables evolve according to a set of coupled governing equations. Our focus is on the following canonical form,

$$\begin{cases} \mathcal{R}(p, s) = \frac{\partial}{\partial t} a(p, s) - \nabla \left[\mathbf{k}(p, s) \nabla p \right] + w(x, t) = 0 & \mathbf{x} \in D \subset \mathbb{R}^3, \ t \geq 0, \\ \mathbf{k}(p, s) \nabla p = 0, & \mathbf{x} \in \partial D, \ t \geq 0, \\ (p, s) = \left(p^0, s^0 \right), & \mathbf{x} \in D, \ t = 0, \end{cases} \tag{2.1}$$

where $\mathcal{R}$ is the general nonlinear residual operator. The accumulation term, a, is generally

nonlinear and it incorporates a heterogeneous porosity and general density dependencies. The mobility function, $\mathbf{k}$, incorporates a spatially varying permeability tensor and a dynamic mobility dependency. The net source term is denoted as w, and it may be spatially and temporally variable. Finally, the auxiliary conditions in Equation 2.1 prescribe a no-flow outer boundary condition and a compatible initial condition.

The three nonlinear functional terms appearing in the governing equations (accumulation, mobility, and net sources) are generally functions of both state variables. This fact leads to the nonlinear coupling between the flow and transport. An approximation to the solution of the coupled system is often obtained by sequentially isolating the pressure and transport components (see for example. [4]). This is accomplished by successively freezing the functional dependencies; for example $a(p, s)$ is considered as $a(p)$, with a frozen saturation state, s, that becomes a parameter rather than a variable. In one iteration of this strategy, transport is frozen and a decoupled pressure is obtained. The new pressure is subsequently frozen and an updated transport variable is obtained. The sequential strategy continues with such iterations until convergence.

The general form of the flow equation with frozen transport terms is,

$$\begin{cases} \mathcal{R}_{\mathcal{F}}(p) = \frac{\partial}{\partial t} a(p) - \nabla \left[\mathbf{k}(p) \nabla p \right] + w(x,t) = 0 & \mathbf{x} \in D \subset \mathbb{R}^3,\ t \geq 0, \\ \mathbf{k}(p) \nabla p = 0, & \mathbf{x} \in \partial D,\ t \geq 0, \\ p = p^0, & \mathbf{x} \in D,\ t = 0, \end{cases} \tag{2.2}$$

The transport equation on the other hand is,

$$\begin{cases} \mathcal{R}_{\mathcal{T}}(s) = \frac{\partial}{\partial t} a(s) - \nabla . \mathbf{f}(s) + w(x,t) = 0 & \mathbf{x} \in D \subset \mathbb{R}^3,\ t \geq 0, \\ \mathbf{f}(s) . \hat{\mathbf{n}} = 0, & \mathbf{x} \in \partial D,\ t \geq 0, \\ s = s^0, & \mathbf{x} \in D,\ t = 0, \end{cases} \tag{2.3}$$

2.1 Example: Locality in compositional Enhanced Oil Recovery

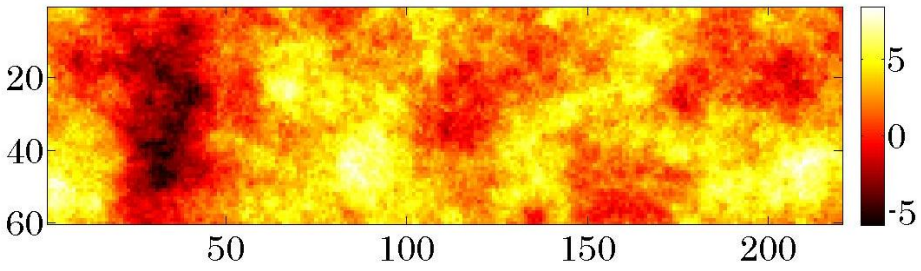


Figure 1: A plot of the logarithm of permeability taken from the tenth layer of the SPE 10 model [13].

Consider a spatial domain that is a two-dimensional horizontal field. The permeability, and the correlated porosity, are taken from the tenth layer of the SPE 10 Comparative Study Model [13]and Figure 1 shows a plot of the logarithm of permeability throughout the field. The spatial domain is discretized using a 60 by 220 Cartesian mesh. We will consider a scenario that is modeled by the flow of four chemical components each of which may partition into the oil and gas phases. The field is operated under a gas injection Enhanced Oil Recovery process. In this process, four production wells are operated at each corner of the domain while one injection well is operated in the center of the field. The injection well is operated under a Bottom Hole Pressure (BHP) constraint of 1828-psi and it injects a gaseous mixture of Methane and Carbon Dioxide into the reservoir accordingly. The production wells are operated under a fixed BHP control of 435 psi. At the beginning of the process, before any fluids are produced or injected, the uniform reservoir pressure is 1100 psi.

In this system, there is one flow variable and it is the pressure distribution throughout the reservoir. There are four transport variables of which one is the gas saturation. This system is modeled by Equation 2.1, with a specific choice for the accumulation, flow, and source functions [4, 12]. There is considerable compressibility in the system owing to the presence of the gas phase.

Figure 2 shows a sequence of three time snapshots of the pressure and gas saturation distribu-

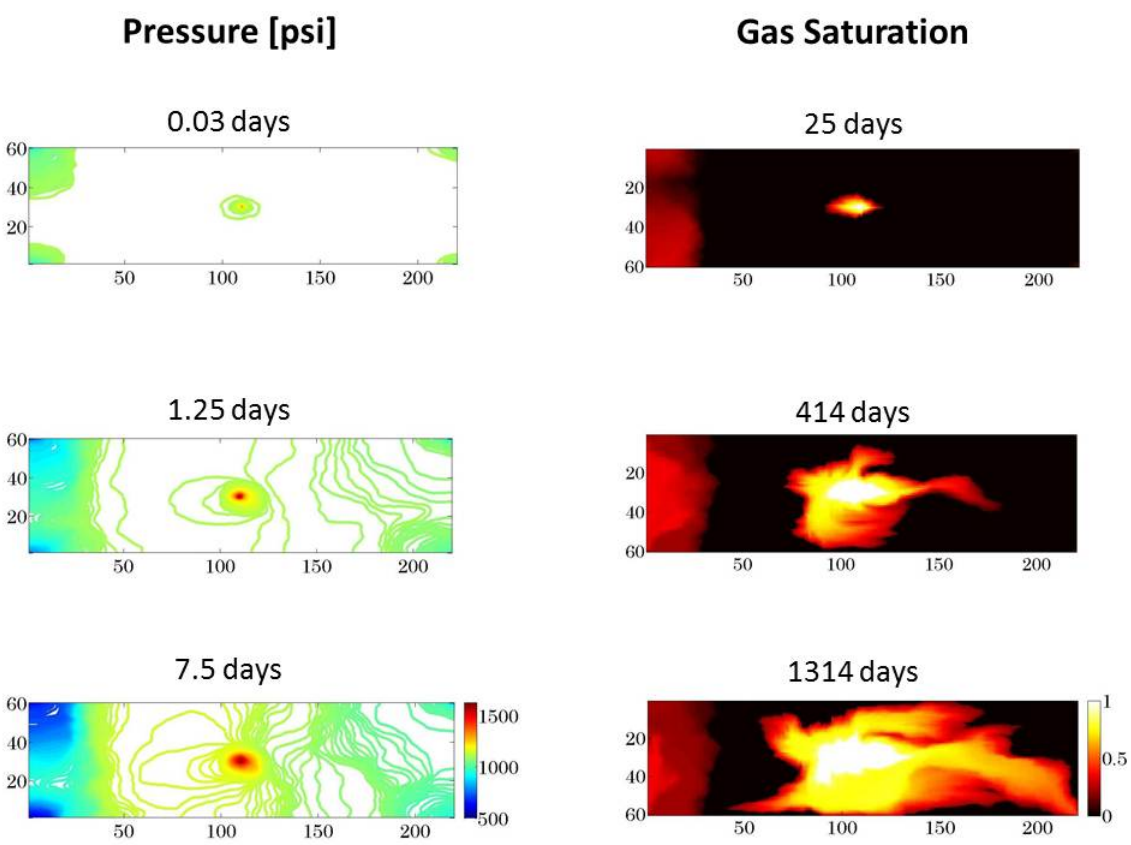


Figure 2: Pressure contour and Gas Saturation snapshots at different times during the course of a compositional multiphase simulation

tions throughout the field. The time associated with each snapshot is indicated in the figure. The reservoir is initially pressurized such that the original fluid within it is in the oil phase exclusively. As gas is injected and the production wells come online, a pressure gradient develops. Because of the structure of the permeability in this example, the two production wells on the left side of the domain draw down a steeper gradient. This introduces a rather substantial phase change from oil to gas due to thermodynamic stability. Forced gas phase introduction occurs due to direct injection, and in this case, the injected gas produces an asymmetric front.

Upon inspection of the pressure snapshots in Figure 2, a number of observations can be made pertaining to the instantaneous spatiotemporal support of changes in pressure. First, at early times, owing to the compressibility in the system, there is a clear locality in δ_p centered at the wells

and propagating outwards over time. The locality gives way to a global evolution as the pressure waves interact with each other and with the domain boundaries. The timescale for the dissipation of spatiotemporal locality in this example is on the order of hours. The flow component is therefore clearly evolving at a fast rate. On the other hand, upon inspection of the saturation profiles, we see a distinct travelling wave character. The locality in the support of the instantaneous changes, δ_s, is governed by the nonlinear wave dynamics as well as by the underlying heterogeneity. Locality is preserved over a timescale that is on the order of years.

2.2 The basic question

In a system that can be modeled by one of the canonical forms (Equations 2.1 through 2.3), what is the instantaneous spatiotemporal support of the flow and transport variables, and what parameters does it depend on?

Mathematically, at any given instant in time, $t \geq 0$, suppose that we are informed of the present states of the system; $p\left(x \in D, t\right)$ and $s\left(x \in D, t\right)$. We are interested in an infinitesimal time increment, $\epsilon > 0$. Particularly over this time increment, the instantaneous change in flow is,

$$\delta_p = \left\| p\left(x, t+\epsilon\right) - p\left(x, t\right) \right\|,$$

and that in transport is,

$$\delta_s = \left\| s\left(x, t+\epsilon\right) - s\left(x, t\right) \right\|.$$

We are seeking to characterize the set of points that are in the spatiotemporal support for the change in flow,

$$\Omega_p = \operatorname{supp}\left(\delta_p\right),$$

and in transport variables,

$$\Omega_s = \operatorname{supp}\left(\delta_s\right).$$

Equations 2.1 are coupled, time-dependent, and generally nonlinear Partial Differential Equations (PDE) that are of mixed order in space. There is no hope for an analytical solution in the general canonical case [18]. Instead, it may be more analytically tractable to derive sharp estimates $\hat{\delta_{p,s}}$ such that,

$$\hat{\delta_{p,s}} \geq \delta_{p,s} \geq 0,$$

and subsequently we would have a conservative estimate of the support set since,

$$\Omega_{p,s} \subseteq \tilde{\Omega}_{p,s} = \operatorname{supp} \hat{\delta_{p,s}}.$$

The definitive characterisation of the support sets, $\Omega_{p,s}$, or their estimated supersets, $\tilde{\Omega}_{p,s}$ is no trivial task. To date, there is no analytical characterization available for the canonical form.

3 The proposed approach

The proposed approach is analytical and leads to numerical, sharp, and conservative *a priori* estimates of the spatial support of instantaneous changes in flow and transport. In this section, we first develop the approach for an abstract system. We then present a specific application of the approach to general flow in one-dimension.

3.1 Analytical overview

We will study the evolution of a system of independent state variables,

$$u(\mathbf{x}, t) : \Omega \subseteq \mathbb{R}^N \times \mathbb{R}^+ \to \mathbb{R}^M.$$

We will restrict our attention to systems that are governed by the general form,

$$\mathcal{R}(u) = \frac{\partial}{\partial t} a(u) + \mathcal{F}(u, \nabla u, \Delta u),$$

that is augmented with compatible auxiliary conditions. The task at hand is the following: given the present state, $u(\mathbf{x}, t)$, deduce the spatial support of the instantaneous change in state over an infinitesimal time increment $\Delta t > 0$. That is, we aim to deduce

$$\operatorname{supp}(\delta_{\Delta t}) \subseteq \Omega,$$

where the instantaneous change in state is defined as,

$$\delta_{\Delta t} = |u(\mathbf{x}, t + \Delta t) - u(\mathbf{x}, t)|.$$

We can accomplish this by first studying the fully-implicit, temporally semidiscrete approximation. Let the temporally discrete starting state be $u^0(\mathbf{x}) = u(\mathbf{x}, t)$. Then the state snapshot at $t + \Delta t$ is denoted

$$u^1(\mathbf{x}) \approx u(\mathbf{x}, t + \Delta t),$$

and it satisfies the system of equations,

$$\mathcal{R}\left(u^1\right) = a\left(u^1\right) - a\left(u^0\right) + \Delta t \mathcal{F}\left(u^1, \nabla u^1, \Delta u^1\right) = 0. \tag{3.1}$$

The equation above is generally nonlinear and with varying coefficients. A general analytical solution is not available. Instead of trying to solve the equation directly, we will apply an iterative method: Newton's Method [16]. The iterative process will generate a sequence of functions

$$\left[u^1\right]^{(\nu)}(\mathbf{x}), \qquad \nu = 0, 1, 2, \ldots,$$

that ultimately converges to the new state;

$$\lim_{\nu\to\infty}\left[u^1\right]^{(\nu)} = u^1(\mathbf{x}).$$

The starting point for the iteration is simply the present state,

$$\left[u^1\right]^{(0)} = u^0(\mathbf{x}),$$

and the iterates are generated using the Newton Updates,

$$\delta^{(\nu+1)} \equiv \left[u^1\right]^{(\nu+1)} - \left[u^1\right]^{(\nu)}, \qquad \nu = 0, 1, 2, \ldots,$$

which are obtained as the solutions to the **linear differential equations**,

$$\mathcal{R}'\left(\left[u^1\right]^{(\nu)}\right)\left(\delta^{(\nu+1)}\right) = -\mathcal{R}\left(\left[u^1\right]^{(\nu)}\right), \tag{3.2}$$

where $\mathcal{R}'\left(\left[u^1\right]^{(\nu)}\right)\left(\delta^{(\nu+1)}\right)$ is the generalized Fréchet derivative of the residual system of equations that is evaluated at the current iterate, $\left[u^1\right]^{(\nu)}$, and applied onto the Newton update, $\delta^{(\nu+1)}$. The derivation of the Fréchet derivative for general operators is often referred to as *quasilinearizaiton* as it produces an operator that is nonlinear in the current state but that is linear in the unknown Newton update. For the functional forms of the PDEs that we are focused on, Equation 3.2 is invariably of the form,

$$f(\mathbf{x})\,\Delta\delta^{(\nu+1)} + g(\mathbf{x})\,\nabla\delta^{(\nu+1)} + h(\mathbf{x})\,\delta^{(\nu+1)} = -\mathcal{R}\left(\left[u^1\right]^{(\nu)}\right), \tag{3.3}$$

where the variable coefficients f, g, and h are general functions of the current iterate, $\left[U^1\right]^{(\nu)}(\mathbf{x})$, and its spatial derivatives. While Equation 3.3 is linear in the Newton update, it involves variable coefficients. This variability is due to the fact that the coefficients depend on the old iterate and on

the underlying heterogeneity that is in the original PDE. Assuming that Equation 3.3 can be solved at each iteration $\nu = 0, 1, \ldots$ the Newton sequence of updates is generated.

Finally, notice that provided that the iteration converges, we have obtained an estimate of the instantaneous change in state over the time increment Δt. It is simply,

$$u^1 - u^0 = \delta_{\Delta t} \equiv \sum_{\nu=1}^{\infty} \delta^{(\nu)}.$$

A conservative estimate of its support is readily obtained in terms of the individual supports of the updates,

$$\text{supp}\,(\delta_{\Delta t}) \subseteq \cup_{\nu=1}^{\infty} \text{supp}\left(\delta^{(\nu)}\right).$$

3.1.1 Solution strategies for the quasilinear Newton update problem

The Newton sequence is generated by successively solving Equation 3.3. While the equation is linear, it generally has spatially varying coefficients. Subsequently, it may not be possible to obtain closed form analytical solutions for the Newton update at each iteration. Just as in Newton's method for the solution of algebraic systems of equations, it is the solution of the linear update problem that is the main work kernel. In the solution of large-scale algebraic linear systems, often indirect and preconditioned methods are used to obtain estimates of the Newton update. Analogously, for our present purpose, we will seek conservative, and yet sharp, estimates for the Newton update, $\hat{\delta}^{(\nu)}$, such that it satisfies,

$$\left|\hat{\delta}^{(\nu)}\right| \geq \left|\delta^{(\nu)}\right|. \tag{3.4}$$

Consequently, it is easy to obtain a superset of the nonzero support of the change, since,

$$\text{supp}\left(\hat{\delta}^{(\nu)}\right) \supseteq \text{supp}\left(\delta^{(\nu)}\right). \tag{3.5}$$

There are two strategies to generate estimates that satisfy Equation 3.4. One deals with analytically homogenizing the variable coefficients f,g, and h, and the other exploits linearity and superposition in order to locally homogenize the residual term.

The analytical homogenization of the variable coefficients within the Fréchet derivative in Equation 3.3 can be as simple as taking the supremum of infimum of the coefficient, e.g.

$$f^* \equiv \sup_{\mathbf{x}\in\Omega} f(\mathbf{x}).$$

Other tactics include taking the volume average of porosity over the domain or the harmonic average of permeability. These tactics recast the linear differential equation into a form with constant coefficients;

$$f^*\Delta\hat{\delta}^{(\nu+1)} + g^*\nabla\hat{\delta}^{(\nu+1)} + h^*\hat{\delta}^{(\nu+1)} = -\mathcal{R}\left(\left[u^1\right]^{(\nu)}\right). \tag{3.6}$$

With an appropriate choice of homogenization strategy, the homogenized Newton update is a sharp upper bound to the original, satisfying Equation 3.4.

A second strategy that is applied exploits the principle of superposition. The residual can be always be written as the sum of $i = 1,\ldots,k$ bump functions, $\phi_i(\mathbf{x})$, each of which has a compact support, $\operatorname{supp}\phi_i(\mathbf{x}) = D_i \subseteq \Omega$, that does not intersect with the support of the other bump functions, $D_i \cap D_j = \emptyset$, $i \neq j$. That is,

$$\mathcal{R}\left(\left[u^1\right]^{(\nu)}\right) = \sum_{i=1}^{k} \phi_i(\mathbf{x}).$$

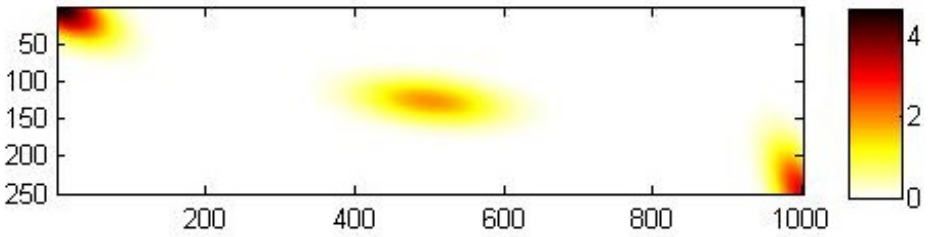
Then, by the principle of superposition Equation 3.6 can be represented as the sum of the sequence of equations,

$$f^*\Delta\hat{\delta}_i^{(\nu+1)} + g^*\nabla\hat{\delta}_i^{(\nu+1)} + h^*\hat{\delta}_i^{(\nu+1)} = -\phi_i(\mathbf{x}), \tag{3.7}$$

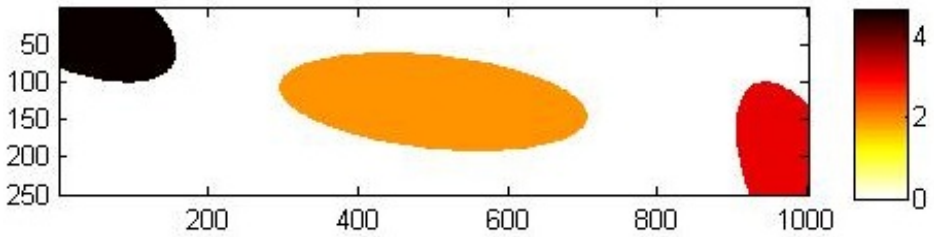
such that

$$\hat{\delta}^{(\nu+1)} = \sum_{i=1}^{k} \hat{\delta}_i^{(\nu+1)}.$$

This decomposition allows us to perform a localized homogenization of the residual. This will be especially useful in situations where the support of the residual consists of the union of a collection of strongly connected components. Consider, for example, the situation depicted in Figure 3. Figure 3a shows a color map of the residual, $\mathcal{R}\left(\left[u^1\right]^{(\nu)}\right)$, for a two-dimensional problem. The support of the residual consists of the union of $k = 3$ compact sets. The homogenization process in this example uses the supremum of each bump function, $\sup_{\mathbf{x}\in\Omega} \phi_i(\mathbf{x})$. The homogenized residual is therefore piecewise constant as depicted in Figure 3b. The principle of superposition may be used to combine the three updates that are due to each bump function.



(a) Color map of the residual.



(b) Homogenized connected components.

Figure 3: The residual evaluated at a hypothetical iteration, $\mathcal{R}\left(\left[u^1\right]^{(\nu)}\right)$

3.1.2 Summary

The analytical process is as follows:

1. Formulate an appropriate set of equations that are semidiscrete in time (Equation 3.1).

2. Derive the Fréchet derivative of the residual semidiscrete operator and write Equation 3.2 in

the form of Equation 3.3.

3. Homogenize the variable coefficients to obtain f^*, g^*, and h^* in Equation 3.6.

4. Decompose the right-hand-side into a collection of local nonzero sets.

5. Solve Equation 3.7 for each $i = 1, \ldots, k$, and sum up the updates.

6. If no homogenization was used, and the residual is not zero, repeat the iterative process until convergence.

3.2 Connections to numerical simulation

The analytical deduction of the support of instantaneous changes in state is connected to the discrete counterpart in numerical simulation. Specifically, the infinite-dimensional and finite-dimensional results are connected through the accuracy of the numerical approximation. Consider a discrete domain, Ω_h, with the discrete state variables $U^n : \Omega_h \subseteq \mathbb{R}^N \to \mathbb{R}^N$. The finite-dimensional approximation to Equation 3.1 is the fully discrete residual system,

$$R_h\left(U^{n+1}\right) = A_h\left(U^{n+1}\right) - A_h\left(U^n\right) + \Delta t F_h\left(U^{n+1}\right) = 0, \tag{3.8}$$

where for some order of approximation, $p \geq 1$, and with appropriate norms, $\|\cdot\|$, the error is formally bounded as,

$$\left\|U^{n+1} - u^n(\mathbf{x})\right\| = O_1\left(h^p\right).$$

Newton's method applied to Equation 3.8 is written as,

$$J_h\left(\left[U^{n+1}\right]^{(\nu)}\right)\Delta^{\nu+1} = -R_h\left(\left[U^{n+1}\right]^{(\nu)}\right), \tag{3.9}$$

where J_h is the Jacobian matrix and the discrete Newton update is defined according to,

$$\left[U^{n+1}\right]^{\nu+1} - \left[U^{n+1}\right]^{\nu} = \Delta^{\nu+1}.$$

It is stated without proof that the fully discrete Newton update, Δ^{ν}, and the infinite-dimensional update, $\delta^{\nu}(\mathbf{x})$, are also related by the approximation accuracy;

$$\|\Delta^{\nu} - \delta^{\nu}(\mathbf{x})\| = O_2\left(h^p\right).$$

Subsequently, in a fully implicit simulation, when a Newton update is to be computed, we may approximate the support of Δ^{ν} by deriving a bound for the support of a corresponding $\delta^{\nu}(\mathbf{x})$. It remains for us to define what that appropriate infinite-dimensional problem needs to be. In this work, we will evaluate the Fréchet derivative of the infinite-dimensional problem using the discrete state and discrete differential operators,

$$\mathcal{R}'\left(\left[U^{n+1}\right]^{(\nu)}, \nabla_h\left[U^{n+1}\right]^{(\nu)}, \nabla_h^2\left[U^{n+1}\right]^{(\nu)}\right).$$

The right hand side of Equation 3.2, will be taken as $R_h\left(\left[U^{n+1}\right]^{(\nu)}\right)$. The form of Equation 3.2 that we will solve to estimate the support at every Newton iteration is,

$$\mathcal{R}'\left(\left[U^{1}\right]^{(\nu)}\right)\left(\delta^{(\nu+1)}\right) = -R_h\left(\left[U^{1}\right]^{(\nu)}\right). \tag{3.10}$$

Figure 4 depicts a fully discrete approximation of the infinite-dimensional residual that appeared in Figure 3. It is important to mention that there are two approaches to the homogenization of the discrete residual. The first approach produces a sharper estimate of the support and it involves solving Equation 3.10 once with a zero right hand side (the homogeneous solution), and as many times as there are grid blocks with nonzero residual entries. The update is then the sum

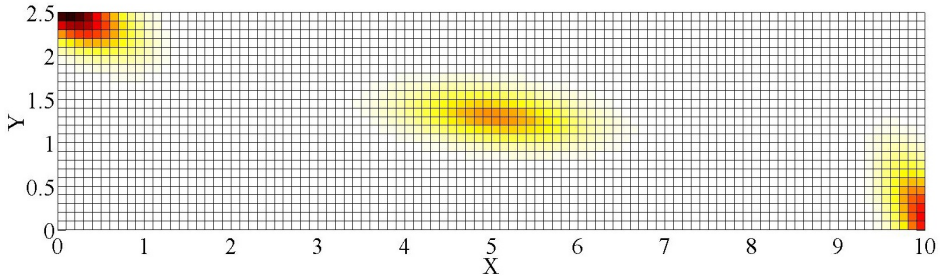


Figure 4: A color map of the discrete residual evaluated at some iteration, ν.

of those individual contributions. The second strategy applies a connected component finding algorithm to isolate and to then homogenize the three sets that appeared in Figure 3b.

3.3 Example: flow in one-dimension

We will consider one-dimensional flow in the domain, $\Omega = [0, 1]$. The canonical form of Equation 2.2 that governs the pressure $p(x, t)$ in one dimension is,

$$\begin{cases} \mathcal{R}_{\mathcal{F}} = \frac{\partial}{\partial t} a(p) - \frac{\partial}{\partial x}\left[k(p)\frac{\partial p}{\partial x}\right] + w(p) = 0 & x \in [0,1],\ t \geq 0, \\ \left[k(p)\frac{\partial p}{\partial x}\right]_{x=0} = 0, & t \geq 0, \\ \left[k(p)\frac{\partial p}{\partial x}\right]_{x=1} = 0, & t \geq 0, \\ p(x,0) = p_{init}(x), & x \in [0,1]. \end{cases} \tag{3.11}$$

1. **Formulate an appropriate set of equations that are semidiscrete in time.** We will apply Backward Euler semidiscretization to Equation 3.11, to obtain,

$$\begin{cases} \mathcal{R}_{\mathcal{F}} = a\left(p^{n+1}\right) - a\left(p^{n}\right) - \Delta t \frac{\partial}{\partial x}\left[k\left(p^{n+1}\right)\frac{\partial p^{n+1}}{\partial x}\right] + \Delta t w\left(p^{n+1}\right) = 0, & x \in [0,1], \\ \left[k\left(p^{n+1}\right)\frac{\partial p^{n+1}}{\partial x}\right]_{x=0} = 0, & , \ n = 0, 1, \ldots, \\ \left[k\left(p^{n+1}\right)\frac{\partial p^{n+1}}{\partial x}\right]_{x=1} = 0 \end{cases} \tag{3.12}$$

with the initial state, $p^0 = p_{init}(x)$.

2. **Derive the Fréchet derivative of the residual semidiscrete operator (Equation 3.12) and write the linear Newton update problem in the form of Equation 3.3.**

The Newton iteration produces the sequence of functions,

$$\left[p^{n+1}\right]^{(\nu+1)} - \left[p^{n+1}\right]^{(\nu)} = \delta^{\nu+1}$$

where the Newton update, $\delta^{\nu+1}$, is obtained as the solution to a linear differential equation. We will introduce the shorthand,

$$p^{(\nu)} \equiv \left[p^{n+1}\right]^{(\nu)},$$

and we note that the iteration is started with the old state as a first guess,

$$p^{(0)} = p^{n}.$$

The Fréchet derivative of the nonlinear operator in Equation 3.12 is,

$$\begin{cases} \mathcal{R}_{\mathcal{F}}{}'\left(p^{(\nu)}\right)\left(\delta^{\nu+1}\right) = \left[a'\left(p^{(\nu)}\right) + \Delta t w'\left(p^{(\nu)}\right)\right]\delta^{\nu+1} - \Delta t \frac{\partial^2}{\partial x^2}\left[k\left(p^{(\nu)}\right)\delta^{\nu+1}\right] & x \in [0,1], \\ \left[\frac{\partial}{\partial x} k\left(p^{(\nu)}\right)\delta^{\nu+1}\right]_{x=0} = 0 & , \ \nu = 0, 1, \ldots \\ \left[\frac{\partial}{\partial x} k\left(p^{(\nu)}\right)\delta^{\nu+1}\right]_{x=1} = 0 \end{cases} \tag{3.13}$$

Provided that $\Delta t k\left(p^{\nu}\right) \neq 0$ we can simplify the Fréchet derivative by introducing the new variable,

$$\hat{\delta}^{\nu+1} \equiv \Delta t k\left(p^{\nu}\right)\delta^{\nu+1},$$

and subsequently, we cab rewrite the linear Newton update problem in the form of Equation 3.3 as follows,

$$\begin{cases} \frac{\partial^2}{\partial x^2}\hat{\delta}^{\nu+1} - h(x)\,\hat{\delta}^{\nu+1} = \mathcal{R}_{\mathcal{F}}(p^{\nu}) \quad x \in [0,1] \\ \left[\frac{\partial}{\partial x}\hat{\delta}^{\nu+1}\right]_{x=0} = 0, \qquad\qquad , \ \nu = 0, 1, \ldots \\ \left[\frac{\partial}{\partial x}\hat{\delta}^{\nu+1}\right]_{x=1} = 0, \end{cases} \tag{3.14}$$

where,

$$h(x) = \frac{a'(p^{\nu}) + \Delta t w'(p^{\nu})}{\Delta t k(p^{\nu})}.$$

3. **Homogenize the variable coefficients in the linear Newton update problem (Equation 3.14) in a way that Equation 3.4 is satisfied.**

   The objective of this step is to homogenize the variable coefficient $h(x)$ in order to recast the differential equation 3.14 into the general form,

$$\frac{\partial^2}{\partial x^2}{\delta_*}^{\nu+1} - h^*{\delta_*}^{\nu+1} = \mathcal{R}_{\mathcal{F}}(p^{\nu}),$$

   where

$$\left|{\delta_*}^{\nu+1}\right| \geq \left|\hat{\delta}^{\nu+1}\right| = \left|\Delta t k(p^{\nu})\,\delta^{\nu+1}\right|. \tag{3.15}$$

   First, we note that depending on the sign of h^*, the linear homogenized problem is either in the form of a screened Poisson equation ($h^* > 0$) or a Helmholtz equation ($h^* < 0$). In the former case, the largest value of the screening coefficient over the domain will produce a conservative solution; i.e. the appropriate homogenization to ensure the condition in Equation 3.4 is,

$$h^* = \sup_{x \in [0,1]} h(x).$$

   On the other hand, the Helmholtz equation produces Newton updates that are oscillatory where the coefficient h^* is the wave number or frequency. We will assume the former case to be true with $h(x) > 0$, $x \in [0, 1]$. Finally, the homogenized linear Newton update problem

becomes,

$$\begin{cases} \frac{\partial^2}{\partial x^2}{\delta_*}^{\nu+1} - \lambda^2 {\delta_*}^{\nu+1} = \mathcal{R}_{\mathcal{F}}\left(p^{\nu}\right) \quad x \in [0,1]\,, \\ \left[\frac{\partial}{\partial x}{\delta_*}^{\nu+1}\right]_{x=0} = 0, \qquad\qquad\qquad\qquad\qquad , \ \nu = 0, 1, \ldots \\ \left[\frac{\partial}{\partial x}{\delta_*}^{\nu+1}\right]_{x=1} = 0, \end{cases} \tag{3.16}$$

where,

$$\lambda = \sqrt{h^*}.$$

The fundamental solution to,

$$\frac{\partial^2}{\partial y^2}\Phi\left(x-y\right) - \lambda^2 \Phi\left(x-y\right) = \delta\left(x-y\right),$$

in the sense of distributions is well known. It is,

$$\Phi\left(x-y\right) = -\frac{1}{2\lambda}\exp\left(-\lambda\left|x-y\right|\right).$$

Subsequently, if we can find a corrector function, $l\left(y;x\right)$, satisfying,

$$\begin{cases} \frac{\partial^2}{\partial y^2} l\left(y;x\right) - \lambda^2 l\left(y;x\right) = 0, \qquad\qquad y \in [0,1] \\ \left[\frac{\partial}{\partial y} l\left(y;x\right)\right]_{y=0} = \left[\frac{\partial}{\partial y}\Phi\left(x-y\right)\right]_{y=0}, \\ \left[\frac{\partial}{\partial y} l\left(y;x\right)\right]_{y=1} = \left[\frac{\partial}{\partial y}\Phi\left(x-y\right)\right]_{y=1}, \end{cases} \tag{3.17}$$

then we can define the Green's function,

$$G\left(x,y\right) = \Phi\left(x-y\right) - l\left(y;x\right),$$

which produces the solution to Equation 3.16 in the form,

$$\delta_*^{\nu+1} = \int_0^1 G(x,y)\,\mathcal{R}_{\mathcal{F}}(p^{\nu}(y))dy. \tag{3.18}$$

In order to solve Equation 3.17, we will first write out the Neumann boundary conditions. Noting that the investigation point is always in the domain, $x \in [0,1]$, we have,

$$\left[\frac{\partial}{\partial y} l(y;x)\right]_{y=0} = -\frac{1}{2}e^{-\lambda x},$$

and,

$$\left[\frac{\partial}{\partial y} l(y;x)\right]_{y=1} = \frac{1}{2}e^{-\lambda(1-x)}.$$

Subsequently, we obtain the corrector function, $l(y;x)$, as,

$$l(y;x) = \frac{1}{\lambda\left(e^{2\lambda}-1\right)}\left[\cosh(\lambda x)\,e^{\lambda y} + e^{\lambda}\cosh(\lambda(x-1))e^{-\lambda y}\right],$$

and the associated Green's function becomes,

$$G(x,y) = \frac{1}{\lambda}\begin{cases}\left[\sinh(\lambda x) - \mu\cosh(\lambda x)\right]\cosh(\lambda y) & \text{if } x \geq y\\ \cosh(\lambda x)\left[\sinh(\lambda y) - \mu\cosh(\lambda y)\right] & \text{if } x < y\end{cases}, \tag{3.19}$$

where,

$$\mu = \frac{e^{2\lambda}+1}{e^{2\lambda}-1}.$$

4. **Decompose the right-hand-side, $\mathcal{R}_{\mathcal{F}}(p^{\nu}(y))$, into the sum of $k \geq 0$ bump functions.**

We are concerned with the effects of a nontrivial residual, $\mathcal{R}_{\mathcal{F}}(p^{\nu}(y)) \neq 0$, for $y \in [0,1]$.

Suppose that the residual consists of the sum of $k \geq 1$ bump functions,

$$\mathcal{R}_{\mathcal{F}}\left(p^{\nu}\left(y\right)\right) = \sum_{i=1}^{k} \phi_i\left(y\right),$$

each of which is supported over a connected interval,

$$D_i = \operatorname{supp}\left(\phi_i\right) = \left[L_a^i, L_b^i\right] \subseteq \Omega.$$

Moreover, we can assume that the intervals are mutually disjoint; $D_i \cap D_j = \emptyset$, for $i \neq j$. Hence, for points within the nonzero support, $y \in \cup_{i=1}^{k} D_i$, the residual is nonzero, and otherwise, it is zero. Finally, we can homogenize each of the constituent bump functions independently. In particular, let the stationary point, y^*, be defined as,

$$y^* = \arg\max_{y \in D_i} \left|\phi_i\left(y\right)\right|,$$

and its corresponding value as,

$$\phi_i^* = \phi_i\left(y^*\right).$$

Then the homogenized form of the bump function is simply,

$$\phi_i^*\left(y\right) = \begin{cases} \phi_i^* & y \in D_i \\ 0 & y \in \Omega - D_i \end{cases}.$$

Finally, the Newton update is obtained as the superposition of solutions,

$$\begin{aligned} \delta_*{}^{\nu+1} &= \sum_{i=1}^{k} \delta_{*i}{}^{\nu+1} \\ &= \sum_{i=1}^{k} \phi_i^* \int_{L_a^i}^{L_b^i} G\left(x, y\right) dy. \end{aligned}$$

5. **Solve for the estimates to the linear Newton updates.**

For the i-th bump function, we can obtain a corresponding Newton update component by integrating the Green's function (Equation 3.19). Because the Green's function is defined piecewise, we need to perform the integral for various situations.

First we will assume that the support of the given right hand side, D_i, is a single point; i.e., $L_a^i = L_b^i = L_*$. In this case, the bump function is a delta distribution, $\phi_i^* \delta(y - L_*)$. The update in this case is simply,

$$\begin{aligned} \delta_*{}^{\nu+1} &= \phi_i^* \int_0^1 G(x,y)\,\delta(y - L_*)dy \\ &= \phi_i^* G(x; L_*)\,. \end{aligned}$$

The analytical formula for the estimate to the update is therefore,

$$\delta_{*,i}^{\nu+1} \approx \frac{\phi_i^*}{\Delta t k(p^\nu)} \frac{1}{\lambda} \begin{cases} [\sinh(\lambda x) - \mu\cosh(\lambda x)]\cosh(\lambda L_*) & \text{if } x \geq L_* \\ \cosh(\lambda x)\,[\sinh(\lambda L_*) - \mu\cosh(\lambda L_*)] & \text{if } x < L_* \end{cases}. \tag{3.20}$$

Next, we will consider cases where the right hand side function has a nontrivial support; $0 \leq L_a^i < L_b^i \leq 1$. In this situation the Green's function integral must be performed assuming three cases; the first assumes that $x \leq L_a^i$, the second assumes that $L_a^i \leq x \leq L_b^i$, and finally , the third that $L_b^i \leq x$. The result is,

$$\delta_{*,i}^{\nu+1} \approx \frac{\phi_i^*}{\Delta t k(p^\nu)} \frac{1}{\lambda^2} \begin{cases} C_1\,[\sinh(\lambda x) - \mu\cosh(\lambda x)] & \text{if } x > L_b^i \\ 1 + \left[\cosh\left(\lambda L_b^i\right) - \mu C_1\right]\cosh(\lambda x) - \sinh\left(\lambda L_a^i\right)\sinh(\lambda x) & \text{if } x\left[L_a^i, L_b^i\right], \\ [C_2 - \mu C_1]\cosh(\lambda x) & \text{if } x < L_a^i \end{cases} \tag{3.21}$$

where,

$$C_1 = \sinh\left(\lambda L_b^i\right) - \sinh\left(\lambda L_a^i\right),$$

and,

$$C_2 = \cosh\left(\lambda L_b^i\right) - \cosh\left(\lambda L_a^i\right).$$

3.3.1 Algorithm in the context of numerical simulation

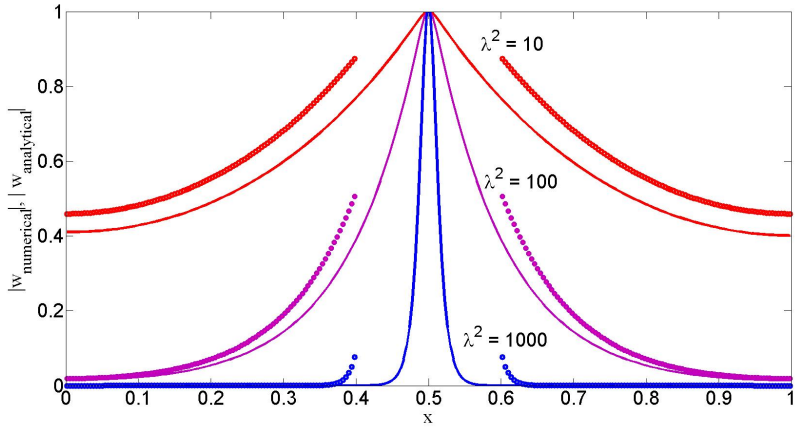


Figure 5: Estimates obtained by an accurate finite difference approximation (solid) and by the proposed method (circle markers) for various values of the screening parameter.

To illustrate the efficacy of the estimate above, we consider a specific case. In this example, the domain is of length $L = 1$, and the screening coefficient is considered uniform. We consider various values for the screening parameter; $\lambda^2 = 10, 100,$ and 1000. The residual at the current iteration is modeled by the bump function,

$$\beta(x) = \exp\left(-\frac{(x-0.5)^2}{1E-04}\right), \tag{3.22}$$

which has a compact support $\Omega = [0.4, 0.6]$. Figure 5 shows the estimates obtained by an accurate finite difference approximation and by the proposed method for various values of the screening parameter. Clearly the proposed estimates are conservative and in this example $\operatorname{supp} w_{numerical} \subseteq$

supp $w_{analytical}$.

4 FuRSST research program on locality

It is hypothesized that the nonzero spatial support of the instantaneous change in state variables can be predicted for the canonical problem (2.1) in multiple dimensions. Moreover, it is conjectured that certain closed form analytical models that depend solely on known parameters of the system provide *a priori* characterizations of the support.

4.1 Mathematical Validation and Analysis

The validation and analysis will follow the approach taken in [46]. For completeness, the approach is summarized in the following section. In the proposed work plan, the approach will be applied to the coupled system in multiple dimensions. The specific proposed work plan is as follows:

1. Extend the analysis in [46] to multiple dimensions for the decoupled flow problem in Equation 2.2.

2. Derive a relation for the decoupled transport problem in Equation 2.3 in multiple dimensions.

3. Derive a relation for the coupled flow and transport transport problem in Equation 2.1.

4. Validate the hypothesis for the SPE 10 model [13].

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