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A sharp analytical bound on the spatiotemporal locality in general two-phase flow and transport phenomena

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Abstract

The objective is to understand, for any two-phase flow situation, the instantaneous spatiotemporal nature of the domain-of-dependence. The focal setting is generally nonlinear and heterogeneous, compressible two-phase flow and transport in porous media. The analytical approach develops a sequence of approximations that ultimately recast the general conservation equations into an infinite-dimensional Newton process. Within this process, the spatiotemporal evolution is dictated by linear differential equations that are easily analyzed. We develop sharp conservative estimates for the support of instantaneous changes to flow and transport variables. Several computational examples are used to illustrate the analytical results.

Keywords: Locality, Nonlinear, Porous Media;

1. Introduction

Nonlinearity and complexity are inherent features in all aspects of the Earth and the Environment. There is a distinct nonlinear stiffness that arises when a process couples various physics that are characterized by different spatiotemporal scales. Specifically, the superposition of physics of disparate characteristic scales brings about a curse of dimensionality. On the one hand, the notion of resolution is limited by the most localized characteristic scale, whereas on the other, the extent of the problem domain is dictated by the most global scale. There is further complexity in such multiscale coupling. The spread of scales and their locality are themselves dynamic, evolving in a nonlinearly complex manner. These aspects of multiscale complexity pose timely challenges in modern forward and inverse modelling methods.

There is no fundamental and universally applicable characterization of the instantaneous spatiotemporal locality of general multiphase flow and transport problems in three-dimensions. Rather, in the literature, there are two approaches to the study of locality. The first approach tackles the general complex problem while devising *ad hoc* estimates. Examples of this occur in the context of adaptive numerical simulation methods that a attempt to exploit locality about travelling waves; for example [1, 2, 3, 4, 5]. In the other approach, limiting cases of idealized problems are studied using exact analytical methods; see for example [6, 7].

This work derives exact analytic results for a general canonical form for multiphase flow and transport while admitting general heterogeneity and nonlinearity.

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1.1. Problem setting

The focus of this work is on the general form of the governing equations for transient two-phase flow in porous media. Following the conventions presented in Appendix A, denote the pressure unknown as, $p(x,t) \in C^2(D \times \mathbb{R}^+)$. Similarly, the transport unknown is labeled as, $s(x,t) \in D \times \mathbb{R}^+$. The two mass conservation governing equations follow the canonical form,

$$\mathcal{R}^{(1,2)}(p(x,t),s(x,t)) = \frac{\partial}{\partial t}a^{(1,2)}(x,p,s) - \nabla \left[\mathbf{k}^{(1,2)}(x,p,s)\nabla p\right] + w^{(1,2)}(x,t) = 0$$
 (1)

$$\mathbf{k}^{(1,2)}\nabla p = 0, \ x \in \partial D, \ t \ge 0, \tag{2}$$

$$(p, s) = (p_{init}, s_{init}), x \in D, t = 0,$$
 (3)

where $\mathcal{R}^{(1)}$ and $\mathcal{R}^{(2)}$ are the general nonlinear residual operators for flow and transport respectively. The accumulation, $a^{(1,2)}$, incorporates a generally heterogeneous porosity and general density dependencies. The mobility functions, $\mathbf{k}^{(1,2)}$, incorporate a spatially varying permeability tensor and a dynamic mobility dependency. The net source terms are denoted as $w^{(1,2)}$, and they may be spatially and temporally variable. Finally, the auxiliary conditions in Equation 1 prescribe a no flow boundary condition and compatible initial conditions.

1.2. Objectives

The objective is to characterize the instantaneous spatiotemporal support of the unknown flow and transport variables. In particular, at any given instant in time, $t \ge 0$, suppose that we are informed of the present states of the system; $p(x \in D, t)$ and $s(x \in D, t)$. In what parts of the spatial domain will the state experience change over an infinitesimal time-step, $\epsilon > 0$?

Denoting the instantaneous changes in state as $\delta_p = p(x, t + \epsilon) - p(x, t)$ and $\delta_s = s(x, t + \epsilon) - s(x, t)$, the questions are answered by characterizing the sets, $\Omega_P = \text{supp}(\delta_p)$ and $\Omega_S = \text{supp}(\delta_s)$. Equations 1 are coupled, time-dependent, and generally nonlinear Partial Differential Equations (PDE) that are of mixed order in space. There is no analytical solution at any given instant for this general case [8]. The objective of this work is to analytically derive sharp estimates $\hat{\delta}_{p,s}$ such that, $|\hat{\delta}_{p,s}| \geq |\delta_{p,s}|$, and subsequently, supp $\hat{\delta}_{p,s} \supseteq \Omega_{p,s}$.

1.3. Outline

In the following section, we proceed by deriving a sequence of related problems that successively cast the problem as one of determining the support of solution to linear, second- and first-order differential equations. This is accomplished by first introducing a sequential solution formulation that allows for the iterative approximation of the dynamic states while treating flow and transport independently. Next, the problem is recast into a semidiscrete implicit form. In this form, the solutions provide the instantaneous changes in state. Finally, infinite-dimensional quasilinearization processes are applied onto the semidiscrete equations, producing the instantaneous state updates as the superposition of a sequence of solutions to linear differential equations. We analyze these differential forms for flow and transport independently in sections 3 and 4, thereby characterizing suitable estimates $\hat{\delta}_{p,s}$. Finally, this is followed by computational examples and a discussion.

2. Recasting the formulation

2.1. Estimates using decoupled flow and transport

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, $\mathcal{R}^{(1)}$, and transport, $\mathcal{R}^{(2)}$, equations.

An approximation to the solution of the coupled system can be obtained by sequentially isolating the pressure and transport components (see for example. [9]). This is accomplished by successively freezing the functional dependencies; for example a(p,S) is considered as a(x,p;s), 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 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,

$$\mathcal{R}^{(1)}(p(x,t)) = \frac{\partial}{\partial t}a(x,p) - \nabla \left[\mathbf{k}(x,p)\nabla p\right] + w(x,t) = 0 \tag{4}$$

$$\nabla p = 0, \ x \in \partial D, \ t \ge 0, \tag{5}$$

$$p = p_{init}, \ x \in D, \ t = 0. \tag{6}$$

The transport equation on the other hand is,

$$\mathcal{R}^{(2)}(s(x,t)) = \frac{\partial}{\partial t}a(x,s) - \nabla [f(x,s)] + w(x,t) = 0$$
(7)

$$f(x,s) = 0, \ x \in \partial D, \ t \ge 0, \tag{8}$$

$$s = s_{init}, \ x \in D, \ t = 0. \tag{9}$$

By considering general solutions to Equations 4 and 7, we can relate to the solution of the coupled system.

2.2. The instantaneous form

In related analytical approaches, time-dependence is often treated by a time-domain transform such as the Laplace transform (see for example [10]). While such approaches recast the equations into steady forms in the transformed domain, any insight gained needs to be translated to the physical domain through an inverse transform. Closed-form inverse transforms to general nonlinear problems are seldom tractable. Since the current focus is on the local, instantaneous nature of the evolution, a fully-implicit [9], semi-discrete form of the governing equations is formed.

The semidiscrete form of Equation 4 becomes,

$$R^{(1)}(p^{n+1}(x)) = A(p^{n+1}) - \Delta_t \nabla \left[K(p^{n+1}) \nabla p^{n+1} \right] + \Delta t W(x, t^{n+1}) = 0, \tag{10}$$

$$\nabla p^{n+1} = 0, \ x \in \partial D, \tag{11}$$

$$p^0 = p_{init}. (12)$$

Over the n^{th} timestep, $t = (n+1) \Delta t$, the solution of the operator equation is the pressure distribution snapshot $p^n(x)$, which is assumed to be unique. The approximation is accurate in the instantaneous limit, $\Delta t \to 0$, and it is a steady governing form for the instantaneous state.

Similarly, the semidiscrete transport equation is,

$$R^{(2)}(s^{n+1}(x)) = A(s^{n+1}) - \Delta_t \nabla F(s^{n+1}) + \Delta_t W(x, t^{n+1}) = 0, \tag{13}$$

$$F\left(s^{n+1}\right) = 0, \ x \in \partial D,\tag{14}$$

$$s^0 = s_{init}. (15)$$

While Equations 10 and 13 are steady PDE, they remain generally nonlinear. Without further specialization to specific nonlinear forms, or to asymptotic subcases (e.g. [11]), it is not possible to directly recast the problem into an equivalent linear one. Instead, in this work, the exact, fully nonlinear form is linearized indirectly using an infinite-dimensional form of a classic result: Newton's Method [12].

2.3. Infinite-dimensional forms for instantaneous state updates

For a general nonlinear residual, $\mathcal{R}\left(u^{n+1}; \Delta t, u^n\right) = 0$, Newton's iterative solution method produces a sequence of iterates $\left[u^{n+1}\right]^{\nu}$, $\nu = 0, 1, \ldots$, that ultimately converge to the solution; i.e. $\left[u^{n+1}\right]^{\nu} \to u^{n+l}$, as $\nu \to \infty$. The sequence starts with the initial guess, $\left[u^{n+1}\right]^{\nu=0} = u^n$. For subsequent iterations, $\nu = 1, \ldots$, the sequence is defined by the analytical solutions to the quasilinear equation,

$$\mathcal{R}'\left(\left[u^{n+1}\right]^{\nu}\right)\left(\left[u^{n+1}\right]^{\nu+1} - \left[u^{n+1}\right]^{\nu}\right) = -\mathcal{R}\left(\left[u^{n+1}\right]^{\nu}\right). \tag{16}$$

In this equation, the operator derivative $\mathcal{R}'(a)(b)$ is the Frechet derivative evaluated at function a and applied onto function b. In the case of algebraic operators, the Frechet derivative is a nonlinear Jacobian matrix evaluated at the vector a and multiplying the vector b.

Note that the Newton update at each iteration, ν , is defined as $\delta^{\nu} = \left[u^{n+1}\right]^{\nu+1} - \left[u^{n+1}\right]^{\nu}$. This means that the instantaneous spatiotemporal change in the state is precisely,

$$\delta = u^{n+1} - u^n = \sum_{\nu=1}^{\infty} \delta^{\nu}. \tag{17}$$

It is the sum of a set of analytical solutions to linear Boundary Value Problems (BVP).

2.3.1. The semilinear flow problem

In the case of flow, we assume that the operator equation, $R^{(1)}(p^{n+1}(x))$, is Frechet differentiable. A sufficient condition for this is that the three coefficient functions, A, K, and W all be differentiable with respect to p^{n+1} . The Frechet derivative of the semidiscrete flow residual evaluated at p, and applied onto function δ_p is,

$$R'(p)(\delta_p) = A'(p)\delta_p - \Delta_t \nabla^2 (K(p)\delta_p). \tag{18}$$

Notice that the Frechet derivative is linear in δ and nonlinear in p. This is why Frechet differentiation is often referred to as a *quasilinearization*. Applying this result, each Newton step, δ^{ν} , is obtained by solving the quasilinearized operator equation,

$$A'(p^{\nu})\delta_{p}^{\nu+1} - \Delta_{t}\nabla^{2}\left(K(p^{\nu})\delta_{p}^{\nu+1}\right) + R^{(1)}(p^{\nu}) = 0, \tag{19}$$

$$\nabla \delta_p^{nu} = 0, \ x \in \partial D, \tag{20}$$

$$\delta_p^0 = 0. (21)$$

2.3.2. The semilinear transport problem

Similar to the development for flow, the Frechet derivative of the transport operator equation $R^{(2)}(s^{n+1}(x))$ evaluated at s, and applied onto function δ_s is,

$$R'(s)(\delta_s) = A'(s)\delta_s - \Delta_t \nabla (F'(s)\delta_s). \tag{22}$$

The Frechet derivative is a first-order linear differential equation in δ_s . Next, we applying this result into the Newton formula to obtain,

$$A'(s^{\nu})\delta_s^{\nu+1} + \Delta_t \nabla \left(F'(s^{\nu})\delta_s^{\nu+1} \right) + R^{(2)}(s^{\nu}) = 0, \tag{23}$$

$$\delta_s^{\nu} = 0, \ x \in \partial D, \tag{24}$$

$$\delta_s^0 = 0. (25)$$

3. Characterizing supp δ_p

The semilinear problem in Equation 19 is in the form of a screened Poisson equation with variable coefficients. The variable coefficient in the second order operator may be eliminated by assuming that $\Delta_t K(p) \neq 0$. In that case, we may make the substitution, $y(x) = \Delta_t K(p^v) \delta_p^{v+1}$. Defining the coefficients, $\alpha(x) = \frac{A'(p^v)}{\Delta_t K(p^v)}$, and $\beta(x) = R^{(1)}(p^v)$, the problem of interest is to characterize the nonzero support of the general form,

$$\Delta y(x) - \alpha(x)y(x) = \beta(x), \tag{26}$$

$$\nabla \left(\frac{y}{K} \right) = 0. \tag{27}$$

The screening coefficient α is generally positive since the derivative of the accumulation with respect to pressure is physically always positive. Let $\lambda = \inf_{x \in D} \sqrt{\alpha(x)} \in \mathbb{R}^+$, and suppose that w(x) is a solution to,

$$\Delta w(x) - \lambda^2 w(x) = \beta(x), \qquad (28)$$

$$\nabla \left(\frac{w}{K}\right) = 0. \tag{29}$$

It then directly follows that $|w(x)| \ge |y(x)|$ for $x \in D$. Equation 28 is now in the form of the screened Poisson equation. The fundamental solution in the sense of distributions is well known. It is,

$$\Phi(x) = \begin{cases}
-\frac{1}{2\lambda} \exp(-\lambda |x|) & x \in \mathbb{R}, \\
-\frac{1}{2\pi} K_o(\lambda |x|) & x \in \mathbb{R}^2, \\
-\frac{1}{4\pi} \frac{\exp(-\lambda |x|)}{|x|} & x \in \mathbb{R}^3
\end{cases}$$
(30)

where K_0 is the modified Bessel function of the second kind and of order zero, and the Euclidean norm of position |x| for $x \in \mathbb{R}^n$ is defined as,

$$r = |x| = \sqrt{\sum_{i=1}^{n} x_i^2}.$$
 (31)

Given domain D with boundary ∂D , it may be possible to construct the appropriate Green's function, $G(x, y) = \Phi(x - y) - h^x(y)$, where $h^x(y)$ is a corrector function satisfying the homogeneous PDE with inhomogeneous boundary data according to the fundamental solution; i.e. it satisfies,

$$\Delta_{y}h^{x} - \lambda^{2}h^{x} = 0, (32)$$

$$\nabla \left(\frac{h^{x}(y)}{K(y)} \right) = \nabla \left(\frac{\Phi(x-y)}{K(y)} \right), \ y \in \partial D.$$
 (33)

Subsequently, the solution to problem 28 is given by,

$$w(x) = \int_{D \subset \mathbb{R}^n} G(x, y) \beta(y) dy$$
(34)

In this paper, we will consider the domain to be the ball of radius l centered at the origin; $B(0, l) = \{x : |x - 0| < l\}$. We are concerned with the influence of compactly supported perturbations in the residual; that is, we consider cases where supp β is compact and is contained in D. The question we are trying to answer can now be rephrased as that of determining supp w. We will obtain a conservative sharp estimate of the support by obtaining an estimate \hat{w} such that $|\hat{w}(x)| \ge |w(x)|$, and subsequently, supp $\hat{w} \ge \sup w \ge D$.

Letting $x \in D \setminus \text{supp}(\beta)$, an estimate is easily obtained as follows:

$$|w(x)| = \left| \int_{y \in \text{Supp}(\beta)} G(x, y) \beta(y) \, dy \right| \tag{35}$$

$$\leq \max_{y \in \text{supp}(\beta)} |\beta(y)| \int_{y \in \text{supp}(\beta)} |G(x, y)| \, dy \tag{36}$$

$$\leq \max_{y \in \text{supp}(\beta)} |\beta(y)| \int_{y \in \text{supp}(\beta)} |\Phi(x - y)| + |h^{x}(y)| \, dy \tag{37}$$

Next, we analytically obtain such estimates for one dimension. Closed form estimates are readily obtained for multiple dimensions using the same process.

3.1. One-dimensional problems

In one-dimension we will treat the domain as the interval D = [0, L] with boundary $\partial D = \{0, L\}$. Assuming that $x, y \in D$, the Green's function for problem 28 is simply,

$$G(x,y) = -\frac{1}{2\lambda(\mu^2 - 1)} \begin{cases} \left(\mu^2 e^{-\lambda x} + e^{\lambda x}\right) \left(e^{-\lambda y} + e^{\lambda y}\right) & \text{if } x \ge y\\ \left(e^{-\lambda x} + e^{\lambda x}\right) \left(\mu^2 e^{-\lambda y} + e^{\lambda y}\right) & \text{if } x < y \end{cases},\tag{38}$$

where,

$$\mu = e^{\lambda} L. \tag{39}$$

In this work, we are concerned with the effects of a nontrivial residual. Suppose that the residual $\beta(x)$ is a bump function with compact support $\Omega = \text{supp}\,\beta(x) = [L_1, L_2] \subset D$. Then for $x \in \Omega$, the residual is nonzero, and for $x \in D \setminus \Omega$ it is zero-valued. Subsequently, estimate (35) allows us to obtain a sharp upperbound on the magnitude of the response w(x) to the residual perturbation with compact support. Performing the simple integrals in the estimates (35), we conclude,

$$|w(x)| \le \max_{x \in \Omega} |\beta(x)| \left| \frac{1}{2\lambda^2 (\mu^2 - 1)} \begin{cases} c_1 \left(\mu^2 e^{-\lambda x} + e^{\lambda x} \right) & \text{if } x \ge L_2 \\ c_2 \left(e^{-\lambda x} + e^{\lambda x} \right) & \text{if } x \le L_1 \end{cases}, \tag{40}$$

where,

$$c_1 = \left(e^{\lambda L_1} - e^{-\lambda L_1}\right) - \left(e^{\lambda L_2} - e^{-\lambda L_2}\right), \text{ and,}$$

$$\tag{41}$$

$$c_2 = \left(e^{\lambda L_1} - \mu^2 e^{-\lambda L_1}\right) - \left(e^{\lambda L_2} - \mu^2 e^{-\lambda L_2}\right). \tag{42}$$

3.1.1. Numerical example 1

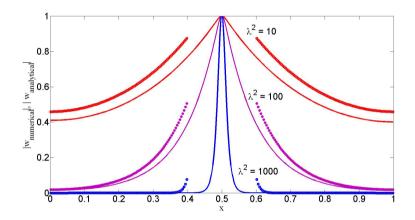


Fig. 1. Estimates obtained by an accurate finite difference approximation (solid) and by the proposed method (circle markers) for various values of the screening parameter.

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,

$$\beta(x) = \exp\left(-\frac{(x - 0.5)^2}{1E - 04}\right),\tag{43}$$

which has a compact support $\Omega = [0.4, 0.6]$. Figure 1 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 supp $w_{numerical} \subseteq \text{supp } w_{analytical}$.

3.1.2. Numerical example 2

4. Characterizing supp δ_s

The transport problem (23) can be recast into a canonical form. We will solve for the variable,

$$v(x) \equiv F'(s^{\nu}) \, \delta_s^{\nu+1}, \tag{44}$$

provided $F'(s^{\nu}) \neq 0$ for $x \in D$. We also define the coefficients,

$$\gamma(x) \equiv \frac{A'(s^{\nu})}{\Delta F'(s^{\nu})},\tag{45}$$

and.

$$\omega(x) \equiv R^{(2)}(s^{\nu}). \tag{46}$$

The semilinear equation for the transport variable Newton iterate is now simply,

$$\nabla v(x) + \gamma(x)v(x) + \omega(x) = 0, \tag{47}$$

$$v(x) = 0, \ x \in \partial D \tag{48}$$

4.1. Example in one-dimension

In one-dimension we will treat the domain as the interval D = [0, L] with boundary $\partial D = \{0, L\}$. Assuming that $x, y \in D$, the general solution has the form,

$$-\frac{\int_0^x e^{\int_0^u \gamma(y) dy} \omega(u) du}{e^{\int_0^x \gamma(y) dy}}$$

$$\tag{49}$$

Clearly, supp $v(x) \subseteq \text{supp } \omega$.

5. Further work

The approach presented in this article can be applied to two and three dimensions, providing sharp conservative estimates of the support of instantaneous spatiotemporal change in two-phase flow and transport phenomena. In this work, one-dimensional results are derived to illustrate the approach. Moreover, this work leads to further analysis into how the spatiotemporal support grows with further infinite-dimensional iterations to convergence. Applications of this approach are anticipated in areas such as the characterization of nonlinear iteration convergence rates for implicit simulation methods, spatially adaptive numerical methods and solvers, and in local time-stepping.

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Appendix A. Conventions and preliminaries

Define the open, bounded spatial domain $D \subset \mathbb{R}^3$ and time $t \in \mathbb{R}^+$. We use discrete counterparts to the spatial and temporal domains. Specifically, for any integer h > 0 we denote the corresponding discrete spatial domain as $D_h = \{x_i \in D : i = 0, 1, ..., h\}$. A discrete temporal domain is defined by the set of times $\{t^n \geq 0 : n = 0, 1, ...\}$, where a time-step is written as $\Delta t^n = t^{n+1} - t^n$.

Lower case letters are used to denote function mappings. For instance, the smooth twice differentiable function $p(x,t) \in C^2(D \times \mathbb{R}^+)$ denotes a transient pressure distribution defined over the spatial domain $x \in D$. Another example is the set of functions representing the semidiscrete pressure distributions for various discrete times; $\{p^n(x): n=0,1,\ldots, \text{ and } x \in D\}$. The spatial *support* of a function, $p(x \in D \to \mathbb{R})$, is denoted as supp (p) and is defined as the set $\omega = \{x \in D: p(x) \neq 0\}$. Outside of its support, a function is identically zero; $p(y \in \mathbb{R}^3 \setminus \omega) = 0$. The function p is said to be *compactly supported* if supp (p) is a compact set.

Vector quantities are denoted by a capital letter and matrices appear in boldface. A subscript indicates that the vector represents quantities that are discretized over space, whereas a superscript denotes a temporally discrete vector. For instance the vector function $P_h(t): \mathbb{R}^+ \to \mathbb{R}^h$ denotes the spatially semidiscrete pressure, and the vector $P_h^n \in \mathbb{R}^h$ denotes a fully-discrete pressure state on the domain D_h at time-step n.

Formally, operators are mappings from one space onto another. We use the term *infinite-dimensional operator* to refer to mappings from one space of functions onto another space of functions; e.g. the divergence operator acting on a smooth function. *Finite-dimensional operators* on the other hand, are mappings from one finite-dimensional vector space on to another; e.g. matrix-vector multiplication. While all functions are formally operators, in this work we reserve the term operator to imply that the domain or the range involve spaces more complex than the real numbers. To emphasize the distinction in each context, operators are italicized. For example, the infinite-dimensional operator $\mathcal{F}(t)(p(x)) = k(t)\nabla p(x)$ is evaluated at point t and is applied onto function p(x), and is a mapping from the space of functions $C^2(D)$ onto the space of vector functions $C(D)^3$. An example of a finite dimensional operator of order h > 0 is $\mathcal{F}_h(t)P_h = \mathbf{K}(t)\nabla_h P_h$, which is an approximation of \mathcal{F} with level of refinement h.

Consider a general infinite dimensional operator, $\mathcal{R}: \Omega \to Y$, that maps from a convex domain $\Omega \subset X$ of a Banach space X onto a Banach space Y. The operator may be Frechet differentiable. A practical method to obtain the Frechet derivative, $\mathcal{R}'(h)(v)$, evaluated at $h \in X$ and applied to $v \in X$, is to set some $h \in X$, and a scalar ϵ , and from the definition of a Frechet derivative, we have,

$$\mathcal{R}'(v)(h) = \lim_{\epsilon \to 0} \frac{\mathcal{R}(v + \epsilon h) - \mathcal{R}(v)}{\epsilon}$$
(A.1)

$$= \left| \frac{d}{d\epsilon} \mathcal{R} (v + \epsilon h) \right|_{\epsilon=0}. \tag{A.2}$$