Numerical solution of ODEs involving the derivative of a Preisach operator and with discontinuous RHS

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Abstract. The purpose of this paper is to numerically solve a special class of ordinary differential equations with discontinuities on the right-hand side and with the Preisach operator under the derivative. We present an algorithm that we devised to numerically integrate this equation making use of a specific approximation from our companion paper, which provided an approximate solution where singularities were expected to occur. We found when the discontinuities forced the right-hand side closer to zero, that the graph of the solution had more parabolic-like curvature similar to the graphs of the solutions using our approximation.

1. Introduction
In this paper we study a model for the discontinuous flow of water through porous media. Such models are of interest in cases where there are almost instantaneous changes in the flow rate, such as when there is switching between precipitation and evaporation in a hydrological system [1]. We can model this using an operator differential equation based on Darcy’s law [2], where the operator models the hysteresis in the system and is known as the Preisach operator, see the companion paper [3] for an introduction. The particular form of this operator ODE is unusual in that the Preisach operator is on the left hand side of the ODE and is under the derivative. These types of Preisach operator ODEs have been the subject of research in [4, 5].

A porous medium is a substance which consists of two or more phases of matter such as solids, liquids and gases. These form a network of pore spaces interconnected by pore throats. Within this network, liquids and gases can move throughout it, but not freely as there is some resistance depending on the type of solid phase. Some examples of porous media are soils, sand, and even biological tissue such as bones. In this paper the porous media of interest to us are soils and the three phases of matter that constitutes a soil are: particles of ground rock or clay, water and air.

Three phase systems of this sort generally exhibit hysteresis in the relationship between moisture content and the capillary pressure. Until recently it was believed that the main cause of this hysteresis was due to the Haines-jumps [6] but nowadays the literature indicates that the contact angle between a liquid and a solid is a more fundamental mechanism [7].

Hysteresis in hydrology has been modeled since the 1930’s by Haines [6], who discovered that the relationship between the soil-moisture content and the capillary pressure was in fact hysteretic. Subsequently Childs and Poulavassilius [8, 9] applied the independent domain model developed by Preisach [10], Néel [11, 12], Everett [13] and others to capillary hysteresis. This was improved upon by Mualem [14, 15, 16] who simplified the model such that only two outer
boundary hysteresis loops were required to determine the inner loops. Parlange improved upon this conceptual model further by reducing the number of required boundary curves to one [17] and this was the approach used by Haverkamp et. al. [18] to fit a series of data from his GRIZZLY database of soils. More recently Flynn et. al. [19] used a one parameter Preisach model to fit this same GRIZZLY data with better accuracy.

The Preisach model [10] was originally conceived for hysteresis in magnetic materials. It was not until the 1970’s that it became a formal mathematical discipline, when Mark Krasnoselskii [20], one of the founders of nonlinear analysis, led an investigation into hysteresis phenomena using the theory of nonlinear operators. This has led to a fertile research area with many papers and monographs being published such as [21, 22, 23]. Not only has the Preisach model been used to model electromagnetism, but it is now used for models in disparate disciplines such as Hydrology [24, 25, 26, 27, 19], Macroeconomics [29, 30], Neural networks [31, 32] and Shape memory alloys [22, 33].

Standard integration algorithms (e.g., Runge–Kutta) are not applicable to operator ODEs because of specific singularities introduced by hysteresis operators. In the previous paper [4] these difficulties have been overcome for systems with a Preisach operator under the derivative and a smooth right-hand side. It was suggested that in addition to standard integration steps, special “linear” steps should be made at certain moments. In this paper we consider equations with a right-hand side discontinuous in time, and we suggest a new technique, which we call “square-root” step, to adapt the previously published algorithm to the discontinuous case. In the companion paper [3] we discuss the questions of existence and uniqueness of a solution of the equation in question, and we also prove a theorem which describes the behaviour of the solution at the points of discontinuities of right-hand side. This theorem provides reasoning for the “square-root step” method. For a simple explanation of the “square-root” step refer to section 5 of the companion paper [3].

The paper is organised as follows. In section 2 we describe the equations that we are interested in. Section 3 describes the physical problem that we wish to model namely the flow of liquids through porous media. Then in section 5 we present an algorithm to numerically solve this type of equation and in section 4 results of numerical simulations will be shown. Finally some conclusions will be drawn in section 6.

2. Equation with discontinuity
Consider the following differential-operator equation

\[ \frac{dP(x(t))}{dt} = f(t, x(t)), \quad (1) \]

where \( f \) is a smooth function and \( P \) is the Preisach operator, for a description see [4] or [3]. Now we consider the addition of an extra term to the right hand side of equation (1) as follows.

\[ \frac{dP(x(t))}{dt} = f(t, x(t)) + g(t) = F(t, x(t)), \quad (2) \]

This extra term, \( g(t) \) is a discontinuous function in time only. From now on we will work with a simple discontinuous function where the points of discontinuity are known in advance, such as

\[ g(t) = \text{sgn}(\cos(n\pi t)), \quad (3) \]

where \( n \) determines the frequency of the jump discontinuities.

Even though this is a very simple type of discontinuity (see figure 1), it can be used to model a number of physical systems, e.g. the switching between raining and drying in a hydrological
system. This trivial function still presents a nontrivial problem to solve (2) numerically due to the discontinuity.

In [4] discontinuities in the right hand side were avoided, now a means to numerically solve equations such as equation (2) will be presented.

\[
g(t) = \frac{1}{1 + e^{-t}}
\]

Figure 1. The figure on the left is an example of a simple discontinuity \( g(t) \). The figure on the right is a modulated sinusoid with the jumps from the left figure included as described by the function \( F(t, x(t)) \). The arrows indicate the location and direction of the discontinuous jumps.

3. Physical system to be modelled

Flows through unsaturated porous media are usually assumed to satisfy three conditions

1. conservation of water mass, or of water volume when the density is constant,
2. a non-linear potential flow obeying a generalised Darcy Law,
3. a rate-independent relationship between water content and potential which closes the system of equations that express the first two conditions.

It is widely known from experiment that such unsaturated flows are hysteretic [18, 19]. In the past, hysteretic flows have either been avoided by considering non-reversing flows, or by treating flow-reversal in an ad hoc manner. The integration of this hysteretic system is explored in this paper using a simplified case where there is no spatial variation—the zero-dimensional case.

The dimensionless ‘volumetric water content’, \( \theta \), is defined to be the volume of water per volume of block of “soil-solids, water and air”. \( \theta \) is zero when the soil is completely dry; \( \theta \) is maximum, less than one, when the block is saturated with water and no air is present. The specific volumetric flow rate of water \( q \) into or out of the block is the volumetric flow per volume of block. Flow into the block is positive; flow out of the block is negative.

Conservation of the volume of water in the block requires the rate of change of the volumetric water content to equal the specific flow at all times. It is expressed as follows:

\[
\dot{\theta} = q, \quad \theta(0) = \theta_0, \quad 0 \leq \theta \leq \theta_s < 1.
\]

Since spatial variation is excluded, the generalised Darcy Law says in this case that the instantaneous specific flow depends on the difference between the potential energy per unit mass of water in the block and a reference value outside the block. When there is no difference in the vertical position of water inside and outside the block, the gravitational potential plays no role. Only the difference in the matric, or capillary, potential drives the flow. Consequently,

\[
q = -k \left( \psi(\theta) - \psi_{\text{ref}}(t) \right),
\]
where \( k \) is the hydraulic conductivity of the medium, \( \psi_{\text{ref}}(t) \) is a time dependent reference potential, \( \psi(\theta) \) is the matric potential at a given moisture content \( \theta \) and is defined by Campbell [34] as: the amount of work, per unit mass of water, required to transport an infinitesimal quantity of soil solution from the soil matrix to a reference pool of the same soil solution at the same elevation, pressure and temperature.

Both the hydraulic conductivity and the matric potential may exhibit hysteresis. There are a number of possible choices for further simplification of expression (5). In the first and most simple case, the rate-independent relationship \( q = -k \theta \) (the so-called linear reservoir of hydrological theory) can be made hysteretic by replacing \( k \) with a Preisach operator. An examination of the hysteretic linear reservoir is reported in [26, 27]. In this paper, \( k \) is taken as a constant and a realistic Preisach operator models the relationship between matric potential and volumetric water content.

The combined ODE and Preisach operators exhibit non-local memory. See [28] for a discussion of non-local memory and rate independence, which are the key characteristics of dynamic hysteretic systems. The existence of two return-points in the non-local memory, completely dry and saturated respectively, ensure predictability.

For the reference potential we will choose the same reference potential \( \psi_{\text{ref}}(t) \) as in [4], but this time we will include an extra term \( g(t) \) for the discontinuity. Thus the reference potential will be a time-dependent sinusoidal driving function with an additional discontinuous time dependent function

\[
\psi_{\text{ref}}(t) = -A \left( 1 + \cos \left( \frac{2\pi t}{T} \right) + \cos \left( \frac{\pi t}{\sqrt{2}T} \right) + g(t) \right),
\]

where \( A > 0 \) is the amplitude, \( T \) is the period and \( g(t) = \text{sgn}(\cos(t)) \). Note that this function satisfies the condition of always being non-positive.

If we combine equations (6) and (5) and substitute them into equation (4), we then have the following:

\[
\dot{\theta}(\psi) = -k \left( \psi(\theta) + A \left( 1 + \cos \left( \frac{2\pi t}{T} \right) \right) + \cos \left( \frac{\pi t}{\sqrt{2}T} \right) + g(t) \right),
\]

\[
\theta(\psi) = P[\psi],
\]

where \( P \) is the Preisach operator [3].

4. Numerical Simulation

In the numerical experiments we solved equation (7) with the following parameter values: \( k = 0.001, A = 20 \) and \( T = 1 \). These were chosen such to cover all possible situations which the algorithm tests for.

The algorithm presented in section 5 was implemented in the C++ programming language. The simulations were performed on a 1.7GHz Pentium Xeon dual-processor PC.

In figure 2 we show two overlayed plots. The solid line is the right-hand side of equation (7) and the dashed line is its solution \( x(t) \), which has been numerically solved by the algorithm. In this figure there are two regions of interest where different parts of the algorithm were dominant. These regions have been magnified in figures 3 and 4 and are discussed below.

- Discontinuous jump in \( F(t, x(t)) \) not crossing t-axis Shown in figure 3 is a magnified view of the region 1 in figure 2. The dashed graph is a plot of the solution \( x(t) \) against \( t \) and the solid graph is a plot of the right hand side, \( F(t, x(t)) \) against \( t \). At the point \( a \), \( F(t, x(t)) \) shows a jump discontinuity, but this does not cross the t-axis. The solution \( x(t) \) at point \( a \), shows a sudden increase in its slope. Likewise a similar situation occurs at point \( b \), where the direction of the jump is reversed and the slope of the solution \( x(t) \) suddenly decreases.
Figure 2. Plot of $F(t,x(t))$ superimposed on plot of $x(t)$ against $t$. Indicated on graph are three regions of particular interest, which are magnified in the following figures.

- Discontinuous jump in $F(t,x(t))$ crossing the $t$-axis Shown in figure 4 is a magnified view of region 2 in figure 2. The dashed graph is a plot of the solution $x(t)$ against $t$ and the solid graph is a plot of the right hand side, $F(t,x(t))$ against $t$. At point a the right-hand side of the ODE, $F(t,x(t))$ shows a jump discontinuity, which does cross the $t$-axis. At this point the normal methods of numerical integration break down and a step known as the "square-root" step is implemented for one step of the program. After this the program starts with a new initial condition and proceeds as normal. The result of this special step, is a parabolic-like curve in the solution and in the right-hand side $F(t,x(t))$ since the solution $x(t)$ is placed back into $F(t,x(t))$. Again a similar situation occurs at point b.

- Discontinuous jump in $F(t,x(t))$ almost crossing the $t$-axis Shown in figure 5 is a magnified view of region 3 in figure 2. The dashed graph is a plot of the solution $x(t)$ against $t$ and the solid graph is a plot of the right hand side, $F(t,x(t))$ against $t$. At point a $F(t,x(t))$ crosses the $t$-axis without any discontinuity. Here the linear-step from [4] is implemented as $F(t,x(t))$ becomes zero when crossing the $t$-axis. At point b the right-hand side of the ODE, $F(t,x(t))$ shows a jump discontinuity, which almost crosses the $t$-axis. It can be observed here that the behaviour of $F(t,x(t))$ and $x(t)$ are quite similar to the case where the discontinuity crosses the $t$-axis, i.e. it has parabolic-like curvature. Note that the "square-root" approximation was not implemented in generating the solution in this case.

5. Algorithm
5.1. General description
The algorithm presented below has been written to solve Preisach operator ODEs of the type shown in equation (2). This algorithm begins at a time $t = t_0$ and will cycle until $t$ reaches a predetermined end time $t = t_{end}$ or if the solution is no longer unique according to proposition 3.1 in [4].
5.1.1. Normal steps  During each cycle a series of checks are performed to determine if the right-hand side of equation (2) changes sign. Special steps are taken when this occurs, these are described below. If there is no special step required, then equation (2) is solved by a numerical integration step $\nu(t_n, x_n, \eta_n; \tau_n)$ where $t_n$ is the current time, $x_n$ is the solution of the ODE as calculated in a previous step, or if there is no previous step it is the initial condition $x_0$. $\eta_n$ is the current state of the Preisach operator and $\tau_n$ is the current time-step to be taken.
5.1.2. Special steps  There are three cases, which can occur where the regular integration method cannot be used. These occur where there is either a change in sign of $F(t, x(t))$ and/or where $g(t)$ has a discontinuity at $t$. The cases which can occur are as follows

(i) $F(t, x) \text{ changing sign and } g(t) \text{ does not have a discontinuity.}$
(ii) $F(t, x) \text{ not changing sign and } g(t) \text{ has a discontinuity.}$
(iii) $F(t, x) \text{ is changing sign and } g(t) \text{ has a discontinuity at } t.$

Case i) is simply the case that was treated in [4]. There, a step known as the “linear step” was taken. It approximated a solution to the ODE, $x_n$, from $t = t_*$ to $t = t_* + h_{linear}$. It then returned to using the numerical integrator with the initial condition $x(t_0) = x_n$, where $t_0 = t_* + h_{linear}$.

Case ii) occurs when a discontinuity in $F(t, x)$ does not cause a change in its sign. This amounts to a sudden change in the slope of the solution. The algorithm determines where this point occurs i.e. when $t = t_*$. It then makes a step of size $t_* - t_n$.

Case iii) requires a special step, which was named the “square-root” step and was derived in a companion paper [3]. As with the other steps mentioned above, the time $t_*$ at which the step is used is determined, in this case by a call to a function GetNextDJump(). The “square-root” step approximates the solution for $x_n$ from $t = t_*$ to $t = t_* + h_{sqrt}$. As with the other special cases, the algorithm returns to using numerical integration with initial condition $x(t_0) = x_n$, where $t_0 = t + h_{sqrt}$.

5.2. Integration algorithm

\begin{verbatim}
integrate1()
    input: Initial values $t_0, \eta_0, x_0$; time step range $[h_{min}, h_{max}]$ and end time $t_{end}$;
    output: Result of the integration is an array of $(t_i, x_i, \eta_i, s_i)_{i=0}^n$
    (1) $n = 0$
    (2) $s_0 = YDirection()$
\end{verbatim}
\( \varsigma = \varsigma_0 \), \( \tau_n = h \)

(4) \( x_{\text{jump}} = \text{GetNextQJump}() \)

(5) \( t_{\text{discon}} = \text{GetNextDJump}() \)

(6) if \( |F(t_n, x_0)| = 0 \)

(7) LinearStep()

(8) \( t_{n+1} = t_n + \tau_n, \quad \eta_{n+1} = \text{UpdatePreisach}(\eta_n, x_{n+1}), \quad n + + \)

(9) while \( t < t_{\text{end}} \)

(10) \( \tau_n = h \)

(11) \( t_{\text{discon}} = \text{GetNextDJump}() \)

(12) \( x_{n+1} = \nu_1(t_n, x_n, \eta_n; \tau_n) \)

(13) if \( (x_n - x_{\text{jump}}) \cdot (x_{n+1} - x_{\text{jump}}) \leq 0 \)

(14) \( \tau_n = \text{JumpToY}() \)

(15) \( x_{\text{jump}} = \text{GetNextQJump}() \)

(16) \( t_{\text{discon}} = \text{GetNextDJump}() \)

(17) else if \( (t_n - t_{\text{discon}}) \cdot (t_{n+1} - t_{\text{discon}}) \leq 0 \)

(18) \( \tau_n = t_{\text{discon}} - t_n \)

(19) \( x_{n+1} = \nu_1(t_n, x_n, \eta_n; \tau_n) \)

(20) if \( F(t_n, x_n) \cdot F(t_{n+1} + \varepsilon, x_{n+1}) \leq 0 \)

(21) \( t_{n+1} = t_n + \tau_n, \quad \eta_{n+1} = \text{UpdatePreisach}(\eta_n, x_{n+1}), \quad n + + \)

(22) SqrtStep()

(23) \( \eta_{n+1} = \text{UpdatePreisach}(\eta_n, x_{n+1}) \)

(24) \( \varsigma_{n+1} = -\varsigma_n, \quad t_{n+1} = t_n + h_{\text{sqrt}}, \quad n + + \)

(25) \( x_{\text{jump}} = \text{GetNextQJump}() \)

(26) \( t_{\text{discon}} = \text{GetNextDJump}() \)

(27) else if \( F(t_n, x_n) \cdot F(t_{n+1}, x_{n+1}) \leq 0 \)

(28) JumpToYP()

(29) \( \eta_{n+1} = \text{UpdatePreisach}(\eta_n, x_{n+1}) \)

(30) \( \varsigma_{n+1} = -\varsigma_n, \quad t_{n+1} = t_n + \tau_n, \quad n + + \)

(31) \( x_{\text{jump}} = \text{GetNextQJump}() \)

(32) LinearStep()

(33) else

(34) \( \varsigma_{n+1} = \varsigma_n \)

(35) \( t_{n+1} = t_n + \tau_n, \quad \eta_{n+1} = \text{UpdatePreisach}(\eta_n, x_{n+1}), \quad n + + \)

GetNextQJump()

**Input:** \( t_n, x_n \)

**Output:** Return value gives the position \( x_{\text{jump}} \) of first discontinuity of \( Q \) in the direction of growth of the solution such that \( Q(x_{\text{jump}}) \neq 0 \).

(1) if \( \varsigma_n = - + 1 \)

(2) if \( K_1 < 3 \) then return \(-\infty\)

(3) else return \( w_n^{(K_1 - 2)} \)

(4) else

(5) if \( K_1 < 3 \) then return \(+\infty\)

(6) else return \( w_n^{(K_1 - 2)} \)

GetNextDJump()

**Input:** \( t_n, \varepsilon \), where \( \varepsilon \) is the smallest possible time step before the discontinuity occurs.

**Output:** Since the discontinuous part of the input is based on the function \( \text{sgn}(\cos(\frac{\pi}{T})) \), where \( T \) is the period, then the jump points will occur at \( t = \frac{\pi m T}{2} \), where \( m \in \{\ldots, 1, 3, 5, \ldots\} \). The return value gives the time \( t_{\text{discon}} \) of the first discontinuity of \( Q \) in the direction of growth of the solution such that \( Q(t_{\text{discon}}) \neq 0 \).
\begin{align*}
(1) & \quad t_{\text{tmp}} = 2t_n/\pi T \\
(2) & \quad \text{if } t_{\text{tmp}} \pmod{2} = 0 \quad \text{then } t_{\text{tmp}} ++ \\
(3) & \quad \text{return } \pi T t_{\text{tmp}}/2 - \varepsilon
\end{align*}

\text{YDIRECTION()}

\textbf{Input:} Current step \( n \)

\textbf{Output:} +1 / -1 if solution is going to increase/decrease

\begin{align*}
(1) & \quad \text{if } F(t_n, x_n) = 0 \text{ and } \frac{\partial F(t_n, x_n)}{\partial t} = 0 \quad \text{then error} \\
(2) & \quad \text{if } F(t_n, x_n) < 0 \quad \text{or} \quad (F(t_n, x_n) = 0 \text{ and } \frac{\partial F(t_n, x_n)}{\partial t} \neq 0) \\
(3) & \quad \text{return } -1 \\
(4) & \quad \text{else} \\
(5) & \quad \text{return } +1
\end{align*}

\text{LINEARSTEP()}

\textbf{Input:} Current step \( n \)

\textbf{Output:}

\begin{align*}
(1) & \quad a = \frac{1}{\rho(x_n, x_n)} \cdot \frac{\partial F(t_n, x_n)}{\partial x}, \quad b = \frac{1}{\rho(x_n, x_n)} \cdot \frac{\partial F(t_n, x_n)}{\partial t} \\
(2) & \quad \text{if } b < 0 \text{ and } \varsigma_n < 0 \\
(3) & \quad x_{n+1} = x_n + (-a - \sqrt{a^2 - 4b}) h_{\text{linear}}/2 \\
(4) & \quad \text{else if } b > 0 \text{ and } \varsigma_n > 0 \\
(5) & \quad x_{n+1} = x_n + (a + \sqrt{a^2 + 4b}) h_{\text{linear}}/2 \\
(6) & \quad \text{else} \\
(7) & \quad \text{error} \\
(8) & \quad \tau_n = h_{\text{linear}}
\end{align*}

\text{SQRTSTEP()}

\textbf{Input:} Current step \( n \)

\textbf{Output:}

\begin{align*}
(1) & \quad c = \sqrt{\frac{2|F(t_n + \varepsilon, x_n) \cdot (t - t_0)|}{\rho(x_n, x_n)}} \\
(2) & \quad x_{n+1} = x_n + \text{sgn}(F(t_n + \varepsilon, x_n)) \cdot c h_{\text{sqrt}}, \quad \varepsilon << t
\end{align*}

\text{JUMPTOY()}

\textbf{Input:} Current step \( n \)

\textbf{Output:} Updated values of \( \tau_n, x_{n+1} \)

\begin{align*}
(1) & \quad \text{Using bisection modify } \tau_n \text{ so that new value } x_{n+1} = \nu_1(t_n, x_n, \eta_n; \tau_n) \text{ satisfies} \\
& \quad |x_{n+1} - x_{\text{jump}}| < 10^{-8}, \ x_{n+1} = x_{\text{jump}} + \zeta \cdot 10^{-8} \cdot x_{\text{jump}} \\
(2) & \quad \eta_{n+1} = \text{UPDATEPREISACH}(\eta_n, x_{n+1})
\end{align*}

\text{JUMPTOYP()}

\textbf{Input:} Current step \( n \)

\textbf{Output:} Updated values of \( \tau_n, x_{n+1} \)

\begin{align*}
(1) & \quad \text{Using bisection modify } \tau_n \text{ so that new value } x_{n+1} = \nu_1(t_n, x_n, \eta_n; \tau_n) \text{ satisfies} \\
& \quad |F(t_n + \tau_n, x_{n+1})| < 10^{-8}
\end{align*}

\text{UPDATEPREISACH}(\eta_{\text{old}}, x)

\textbf{Input:} Old state \( \eta_{\text{old}} \), new input \( x \)

\textbf{Output:} Updated value \( \eta = \{w(i)\} \) and appropriate \( K \)
\begin{align*}
\eta &= \eta_{old}, \quad K = K_{old} \\
\text{if } |x| &> \gamma \\
K &= 1 \\
\text{return } \eta \\
\text{if } x > w(K_{old}) \\
\text{if } K \mod 2 == 0 \text{ then } K &= + 1 \\
\text{while } \ K \geq 3 \text{ and } x > w(K-2) \\
K &= K - 2 \\
\text{else if } x < w(K_{old}) \\
\text{if } K \mod 2 == 1 \text{ then } K &= + 1 \\
\text{while } \ K \geq 3 \text{ and } x < w(K-2) \\
K &= K - 2 \\
\text{if } K \geq K_{max} \text{ then error} \\
w(K) &= x \\
\text{return } \eta
\end{align*}

6. Conclusions

In this paper a toolkit for the numerical solution of Preisach operator ODEs with discontinuities on the right-hand side was presented. It was used to model a simple system from hydrology based on Darcy’s law and a number of interesting features were observed in solutions to this system. One of them was that the solution was more parabolic-like when the discontinuity either crossed or was very close to the t-axis. Although the physical model used to demonstrate the numerical techniques was based in hydrology, the numerical techniques are not limited to this. This algorithm can be used in physical models which satisfy the following conditions:

- The model must be of the general form of equation (2), i.e. with the derivative of the Preisach operator on the left of the ODE.
- When the right-hand side contains a discontinuity, the discontinuity can only be in the time variable [3] and [5].

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