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LAWS

James LaVita

June 1980

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SOME REMARKS ON THE COMPARISON OF METHODS
FOR COMPUTING DISCONTINUOUS SOLUTIONS OF CONSERVATION LAWS

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June 1980

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Abstract

This paper reports on the comparison of some difference schemes for the computation of discontinuous solutions of scalar conservation laws with nonconvex flux terms. Compared are the Random Choice Method, an upwind scheme, a version of Godunov's method and the second order Lax-Wendroff scheme with artificial viscosity term added. For the problems of petroleum reservoir modeling, combustion phenomena and shock detailing, the RCM seems to provide the most useful data.

In recent years some interesting new developments have occurred in the long-standing problem of accurately computing solutions of partial differential equations, primarily systems of hyperbolic conservation laws centering around the so-called Random Choice (or Glimm's) Method. Based on an elegant mathematical construction of Glimm [1965], an efficient and successful computational scheme has been developed by Chorin [1976,1977]. It has been used with satisfying success in the modeling of combustion waves, other kinds of shock phenomena, and in petroleum reservoir modeling by Chorin (see above), Colella [1979], Concus and his co-workers [1979], and others. The problems treated with the Random Choice Method involve Burgers's equation, the Buckley-Leverett equation, and one- and multi-dimensional gas dynamical equations, with and without reacting gas chemistry. As this work progresses it becomes more evident that it is important to know the behavior of computational schemes in the little-understood situations involving non-convexities in the appropriate flux terms of the equations.

Since not many analytical results are known about the systems described above and even fewer concerning the convergence of numerical schemes to the correct entropy producing solutions, it is essential that the behavior of numerical solution methods be tested in situations where some idea of comparative accuracy (in whatever appropriate sense) can be gauged. One goal is to work with the simplest, yet still physically significant, situations and this paper is such an attempt. The results indicate that many phenomena -- such as convergence to non-physical solutions, loss of resolution at shocks, and contact discontinuities -- can be studied, and comparisons can be made for some different methods, but some other phenomena cannot be distinguished well. Thus more delicate experiments

must be conducted. I would like to thank Alexandre Chorin for a variety of illuminating discussions during the course of the work on this paper, and for the original suggestions that led to its initiation.

This paper describes some computational solutions for various schemes, such as Lax-Wendroff, Upwind, Godunov and Random Choice, when applied to a model of the Buckley-Leverett equation, namely

$$u_t + (f(u))_x = 0 \quad u(0, x) = u_0(x) \quad (1)$$

If $\frac{df(u)}{du} = a(u)$, then in regions of smoothness, Eq. (1) is equivalent to $u_t + a(u)u_x = 0$. Eq. (1) appears in the study of the flow of two immiscible fluids through a porous medium in the absence of capillary pressure or gravitational forces. The explicit form of $f(u)$ in the model equation is

$$f(u) = \frac{u^2}{u^2 + \alpha(1-u)^2}.$$

In the case of oil and water, for example, the correct equation is

$$u_t + \frac{Q}{\phi} (f(u))_x = 0$$

where Q is the total flow, ϕ is the porosity, and $f(u) = 1/[1 + \alpha k_0(u)/k_w(u)]$, where $k_0(u)$ and $k_w(u)$ are the relative permeabilities of sand to oil and sand to water respectively; $\alpha = \mu_u/\mu_0$ is a constant, with μ_w and μ_0 the viscosities of water and oil respectively. We refer the interested reader to Concus and Proskurowski [1979] for more details. We take $\alpha = \frac{1}{2}$, $\frac{Q}{\phi} = 1$. Towards the end of the paper, a few preliminary results for a non-monotone, non-convex flux function are described. These show failure to converge to the appropriate entropy preserving solution for all the first order schemes except the Random

Choice Method.

As described in Concus and Proskurowski [1979], the solution of the Riemann problem for Eq. (1) can be given explicitly. In Figure 1 $f(u)$ will be seen to be a monotone: an increasing function of $u \in [0,1]$ with one inflection point (≈ 0.378), dividing a region concave up (on the left) from one concave down (on the right). Here we will describe the solution.

If the chord joining $f(u_L)$ and $f(u_R)$ on the graph does not cross the graph of $f(u)$, the solution is either a shock or a rarefaction. If $a(u_L)$ is greater than $a(u_R)$, there is a shock connecting the state u_L to the state u_R propagating with speed $\frac{dx}{dt} = S_{L,R}$ where

$$S_{L,R} = \frac{f(u_R) - f(u_L)}{u_R - u_L}$$

If $a(u_L)$ is less than $a(u_R)$ then there is an expansion wave connecting u_L and u_R . On the other hand, when the chord cuts the graph of $f(u)$, there are the two cases described below.

In the case where u_L is greater than u_R , construct the convex hull, $H(u)$, to $f(u)$ as shown in Figure 1. The value u_M (≈ 0.556 when u_R is 0.05) is such that

$$S_{M,R} = \frac{f(u_R) - f(u_M)}{u_R - u_M}$$

is exactly equal to $\frac{df}{du}(u_M) = a(u_M)$. Then it is known that the unique piecewise continuous solution for any $u_L > u_R$ is given by:

(I) $u_L \leq u_M$; a shock propagating to the right with speed $\frac{dx}{dt} = S_{L,R}$.

(II) $u_L > u_M$; a shock (contact discontinuity) propagating with speed

$\frac{dx}{dt} = S_{M,R}$ followed by a rarefaction connecting u_M to u_L .

In the case where u_R is greater than u_L , construct the convex hull, $h(u)$, to $f(u)$ as shown in Figure 2.

The general solution is given in great detail in the previous reference.

Section I

In Section I we describe some experiments with the popular Lax-Wendroff scheme, with viscosity, in a 2-step version.

$$u_{j+1/2}^{n+1/2} = \frac{1}{2} (u_{j+1}^n + u_j^n) - \frac{\Delta t}{2\Delta x} (f_{j+1}^n - f_j^n)$$

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x} (f_{j+1/2}^{n+1/2} - f_{j-1/2}^{n+1/2})$$

where $f_e^m = f(u_e^m)$ and then

$$\hat{u}_j^{n+1} = u_j^{n+1} + c \frac{\Delta t}{\Delta x} \Delta_{-1} [|\Delta_{-1} u_{j+1}^{n+1}| \Delta_{-1} u_{j+1}^{n+1}]$$

is the new value. The second term on the right of the last equation is a standard form of the artificial viscosity.

The main result is the construction of Riemann problems for the Buckley-Leverett equation that produce unphysical solutions, i.e., that have expansion shocks. Thus we see that the L-W scheme is an inappropriate tool for use in such standard applications as reservoir modeling unless additional, and no doubt subtle, safeguards can be found. In Figure 3a-d we see the solutions to the problem with data $0.55 = u_L$ and $0.05 = u_R$. Clearly, two shocks are progressing, one with slightly slower

speed. Measurement shows that the speed of the large shock is to within reasonable accuracy what one would get from the jump conditions with $u_L = 0.62$ and $u_R = 0.05$, and the smaller shock is progressing as would a shock with $u_L = 0.55$ and $u_R = 0.62$. The first should have speed approximately 1.46, the second should be 1.18, while the true speed is 1.48. These differences are detectable in the data.

This is equivalent to allowing discontinuities whose chords cut the graph of f , which is not allowed with our choice of u_L, u_R by virtue of known results on uniqueness due to Oleinik. Most significantly a comparison of the computed shock speed for the left and right shocks shows that the computed waves are not just a single wave propagating with the correct speed that happens to exhibit overshoot. Thus this second order method is inapplicable, without further corrective steps being taken, even to the Riemann problem. Other numerical experiments demonstrate that this convergence to the non-physical solution is numerically stable.

Section II

The principle class of difference schemes that can be shown to converge to the physically significant solution is the class of monotone methods. Those results appear, for example, in Harten, Hyman and Lax[1976] and in Crandall and Majda[1980]. Such methods are necessarily of first order. Thus a comparison of the performance of some typical first-order schemes with regard to the sharpness and shape stability of the face is of interest in the useful case of the Buckley-Leverett equation and can give guidance for work on more difficult situations. For example, in combustion

modeling, where the flux functions exhibit several types of non-convexity and even discontinuity, a detailed knowledge of the shape of the face is highly important. It is also not known in general which methods produce the correct physically relevant solutions. In this light any evidence produced by a study of this single non-convex model sheds light on more intractable cases.

Since most variations of the upwind scheme reduce to the simplest for monotone flux functions we have

$$\begin{aligned} u_{\alpha}^{n+1} &= u_{\alpha}^n - \lambda \Delta_x (f(u_{\alpha-1}^n)) u \\ &= u_{\alpha}^n - \lambda (f(u_{\alpha}^n) - f(u_{\alpha-1}^n)) \end{aligned}$$

for the Buckley-Leverett equation. For more complicated flux functions, with stagnation points ($f'(\alpha) = u$) or non-convexities for example, more general schemes, such as that of Majda-Crandall [1980] are needed.

The behavior one hopes for when computing such discontinuities is a sharp or at least a stable profile propagating with the correct speed. Again we ran trials on the model Buckley-Leverett equation with the data $u_L = 0.55$, $u_R = 0.05$. Figure 4 shows the results of computation and the results in the next table are drawn from it. Table 1 lists the width W of the transition zone against number N of steps.

Table 1

N	W
25	8
50	10
75	11

100	12
125	14
150	14
175	15
200	16
225	16
250	16
275	17
300	17
325	18

Of course, one expects this poor behavior because the shock is in fact nearly a contact discontinuity. As shown in our remarks about the solution of the Riemann problem with data $u_R = 0.05$ and u_L greater than u_M , the true unique solution is a contact discontinuity followed by a rarefaction. Unfortunately, in the non-convex case it is just such details of the solution that one would like to see. Trials with a slightly larger value of u_L give results that cannot qualitatively be distinguished from the $u_L = 0.55$ case, and thus important information is lost.

Section III

An attempt to improve the resolving abilities of computational methods can be based on building some features of the exact solutions into the method. Such a method is the one devised by Godunov. A version for one convex scalar equation appears in Majda and Crandall [1980].

The idea of the method is to use the conservation law in integral form

$$0 = \iint u_t + (f(u))_x dA = \int u dx - f(u) d$$

to give an exact value for the integral of $u(x, t + \Delta t)$ between $j\Delta x$ and

$k\Delta x$ and use this to compute some average for u_j^m . The method has the virtue that the solution used in computing the integral is advanced exactly if the Courant-Friedrichs-Lewy condition is satisfied. The process proceeds, following Crandall and Majda, like this. Let data be given as a step function

$$u_0(x) = \sum_{j=-\infty}^{+\infty} u_j^n X_j$$

where $a \leq u_j^n \leq b$, and X_j is the characteristic function of $(j-1/2)\Delta x \leq x \leq (j+1/2)\Delta x$. Now advance the solution $u(x,t)$ exactly by solving

$$u_t + (f(u))_x = 0$$

$$u(x,0) = u_0(x) ,$$

and using the flux balance relation

$$0 = \int_C u dx - f(u) dt$$

where C travels counter clockwise around the box

$$0 \leq t \leq \Delta t , \quad (j-1/2)\Delta x \leq x \leq (j+1/2)\Delta x .$$

We have

$$\begin{aligned} 0 = & \int_{(j-1/2)\Delta x}^{(j+1/2)\Delta x} u(x,0) dx - \int_0^{\Delta t} f(u(j+1/2)\Delta x, t) dt \\ & - \int_{(j-1/2)\Delta x}^{(j+1/2)\Delta x} u(x, \Delta t) dx + \int_0^{\Delta t} f(u((j-1/2)\Delta x, t)) dt . \end{aligned}$$

We now define u_j^{n+1} by the relation

$$u_j^{n+1} = \frac{1}{\Delta x} \int_{(j-1/2)\Delta x}^{(j+1/2)\Delta x} u(x, \Delta t) dx .$$

Thus

$$u_j^{n+1} = u_j^n - \frac{1}{\Delta x} \left(\int_{(j-1/2)\Delta x}^{(j+1/2)\Delta x} f(u((j+1/2)\Delta x, t)) dt - \int_{(j-1/2)\Delta x}^{(j+1/2)\Delta x} f(u((j-1/2)\Delta x, t)) dt \right) .$$

Invoking the Courant-Friedrichs-Lewy condition $|\frac{\Delta t}{\Delta x} \max_{a \leq u \leq b} |f'(u)| \leq 1$, now guarantees that the solution $u((j-1/2)\Delta x, \Delta t)$ is determined by u_{j-1}^n and u_j^n .

The Riemann problem determined by the two values u_{j-1}^n, u_j^n is scale invariant and so $u((j-1/2)\Delta x, t)$ is constant for $0 \leq t \leq \Delta t$. Thus

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x} (f(u((j-1/2)\Delta x, \Delta t)) - f(u((j+1/2)\Delta x, \Delta t)))$$

or in short hand

$$u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x} (f_{j-1/2}^{n+1} - f_{j+1/2}^{n+1}) .$$

An experiment on the same data ($u_L = 0.55$, $u_R = 0.05$) leads to the results shown in Figure 5. One can see that the resolution of the front is qualitatively similar to that of the upwind scheme, not producing a sharp face and smearing the transition region over larger and larger numbers of mesh points. Similarly, experiments with $u_L > u_M$ show that it is difficult to tell the difference between a shock and a contact discontinuity followed by a rarefaction, the solution predicted by the analysis.

Section IV. Random Choice Method

The Random Choice Method (RCM) approximates the solution to (1) by first advancing the solution at each step exactly, as does the Godunov scheme. Then, instead of smearing the solution to obtain the piecewise constant approximation, it samples the solution in an interval and assigns that value to be the new value of the approximation. Success depends on a careful choice of the sampling strategy, and attention to boundaries if they are present. The use of the RCM as a computational tool, as developed by Chorin [1976,1977] and others, was based on a theorem of Glimm [1965] that proved the convergence of the method for strictly nonlinear $f(u)$ (i.e., $\frac{d^2 f}{du^2} \neq 0$) and initial data differing little from a constant. The RCM approaches first order accuracy, as experiment shows, propagates shocks sharply, and is stable. There is some uncertainty introduced by the sampling procedure, limiting, for example, the knowledge of the location of the shock front to be $O(h)$, but this appears to be within acceptable bounds.

Let a_n be an element of a quasirandom sequence. At a given time step t_j the true solution $u(x, t_j)$ is approximated by a step function as in Section III, i.e.,

$$u(x, t_j) \approx \sum_{j=-\infty}^{+\infty} u_j^n x_j,$$

x_j being the characteristic function of $(j - 1/2)\Delta x \leq x \leq (j + 1/2)\Delta x$. One advances to the next time step t_{j+1} in two stages, going first to $t_{j+1/2}$ as follows:

1) Choose $|t_j - t_{j+1}| = \Delta t$ such that the Courant-Friedrichs-Lewy condition

$$\frac{\Delta t}{\Delta x} \max_u |a(u)| < 1$$

to assure that there are no interacting waves.

2) Solve the equation (1) exactly from t_j to $t_{j+1/2}$. This is in fact a series of Riemann problems since there are no interacting waves. Call the solution $w(x, t)$.

3) Construct, as our approximation at $t_{j+1/2}$, the function $v(x, t_{j+1/2})$:

$$v(x, t_{j+1/2}) = \sum_{j=-\infty}^{+\infty} v_{j+1/2}^{n+1/2} y_j$$

where

$$v_{j+1/2}^{n+1/2} = w(j\Delta x + a_m, t_{j+1/2})$$

and y_j is the characteristic function of $j\Delta x \leq x \leq (j+1)\Delta x$.

Notice that the same number a_m is used for all j .

One then proceeds to construct u_j^{n+1} by starting with $v(x, t_{j+1/2})$ at step $t_{j+1/2}$ and advancing to t_{j+1} .

For a_n we choose the van der Corput sequence:

Let

$$\sum_{k=0}^m i_k 2^k = n$$

be the binary expansion of the integer n . Then

$$a_n = \sum_{k=0}^m i_k 2^{-(k+1)}.$$

Figure 6 shows the propagation of the shock front for our data $u_L = 0.55$, $u_R = 0.05$. We see a sharp profile whose position is accurate to within one mesh width of the theoretically computed position.

Section V

The conclusions of our analysis are these. The dangers of convergence to physically false solutions are real in ones even in actual computations. The second order method employed here failed in a typical physically significant case. In the case where the true nature of the solution is more difficult to see, conclusions based on the computed data become even more unreliable. Likewise, the relevance of the computed solution, even in the case where it is known that the computed solution converges to the true physical, as for example in the experiments mentioned before.

The question of the validity of the computation appears even more sharply when we consider examples where nonmonotone schemes are used. Some experimental calculations with the previously valid first order methods on the flux function

$$f(u) = \begin{cases} u^\beta, & 0 \leq u < 0.2 \\ u^\beta + \alpha ff(u), & 0.2 < u < 0.8 \\ u^\beta, & 0.8 \leq u < 1 \end{cases}$$

with $\beta = 1.3$, $\alpha = 3.5$, and $ff(u) = (u-0.2)(u-0.8)$ show interesting results.

The data $u_L = 0.95$, $u_R = 0.05$ leads to a situation where the convex hull joining the function value at 0.95 to the function value at 0.05 requires the solution to consist of two shocks separated by a rarefaction. The convex hull is represented in Figure 7. The shock speeds are given by taking the slopes of the chords of the two linear segments of the hull.

When applied to this problem the upwind method shows severe instability and really can not be compared with the other methods in any useful fashion. The Godunov method and the RCM method are plotted in Figure 8a-d and Figure 9a-d. It is clear that the RCM provides the closest approximation to the theoretical qualitative solution. However, these are preliminary calculations and more evidence is needed in cases of non-monotone, non-convex flux functions.

Thus, of the methods chosen for comparison, the simple tests conducted indicate that the RCM method, though only of first order, promises a superior ability to model accurately the classes of phenomena discussed in the introduction.

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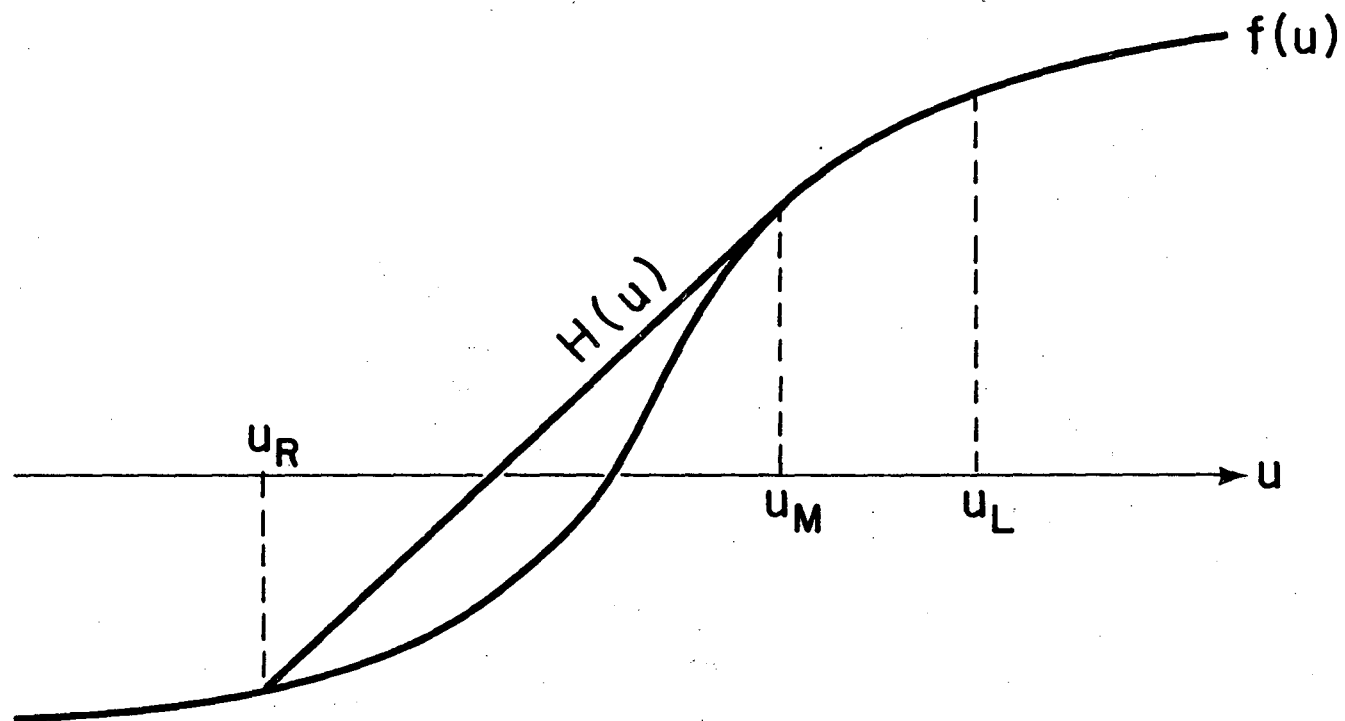
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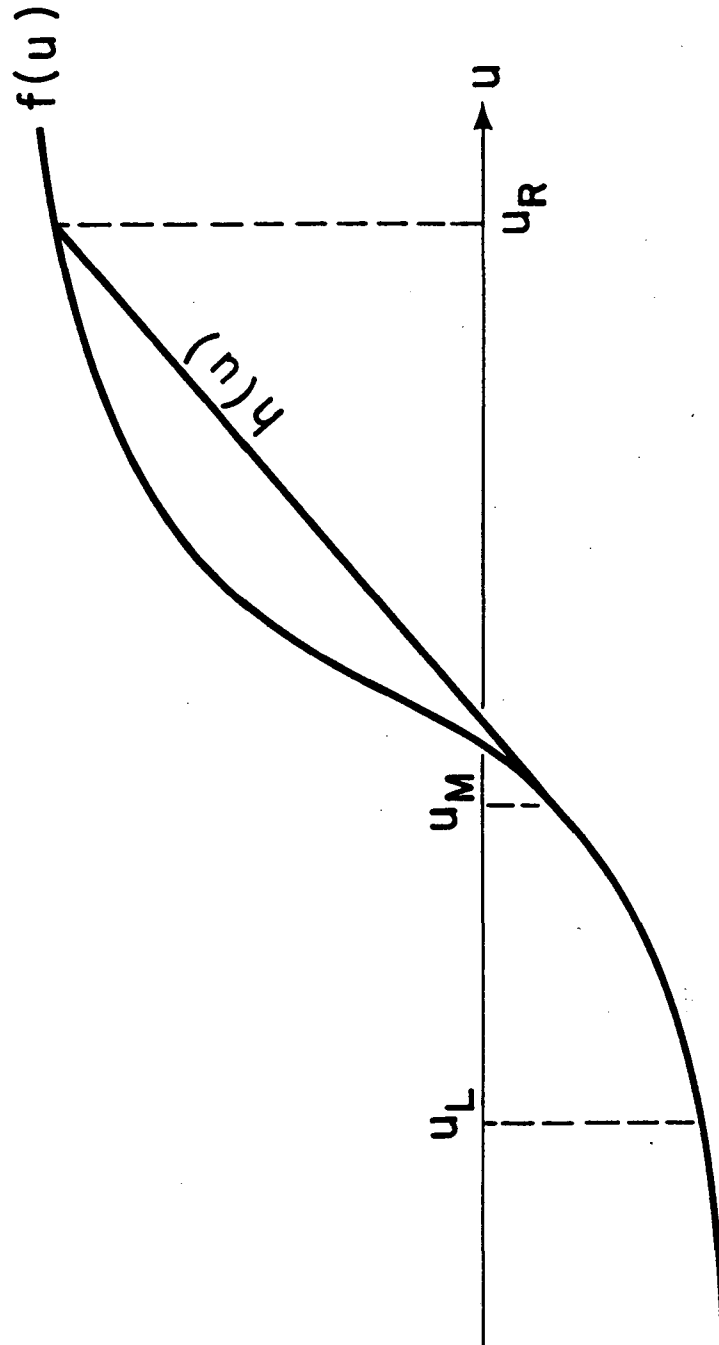
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Figure 1. Shows the function $f(u)$, the point of tangency u_M , and the convex hull $H(u)$.



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Figure 2. Shows the convex hull $h(u)$.

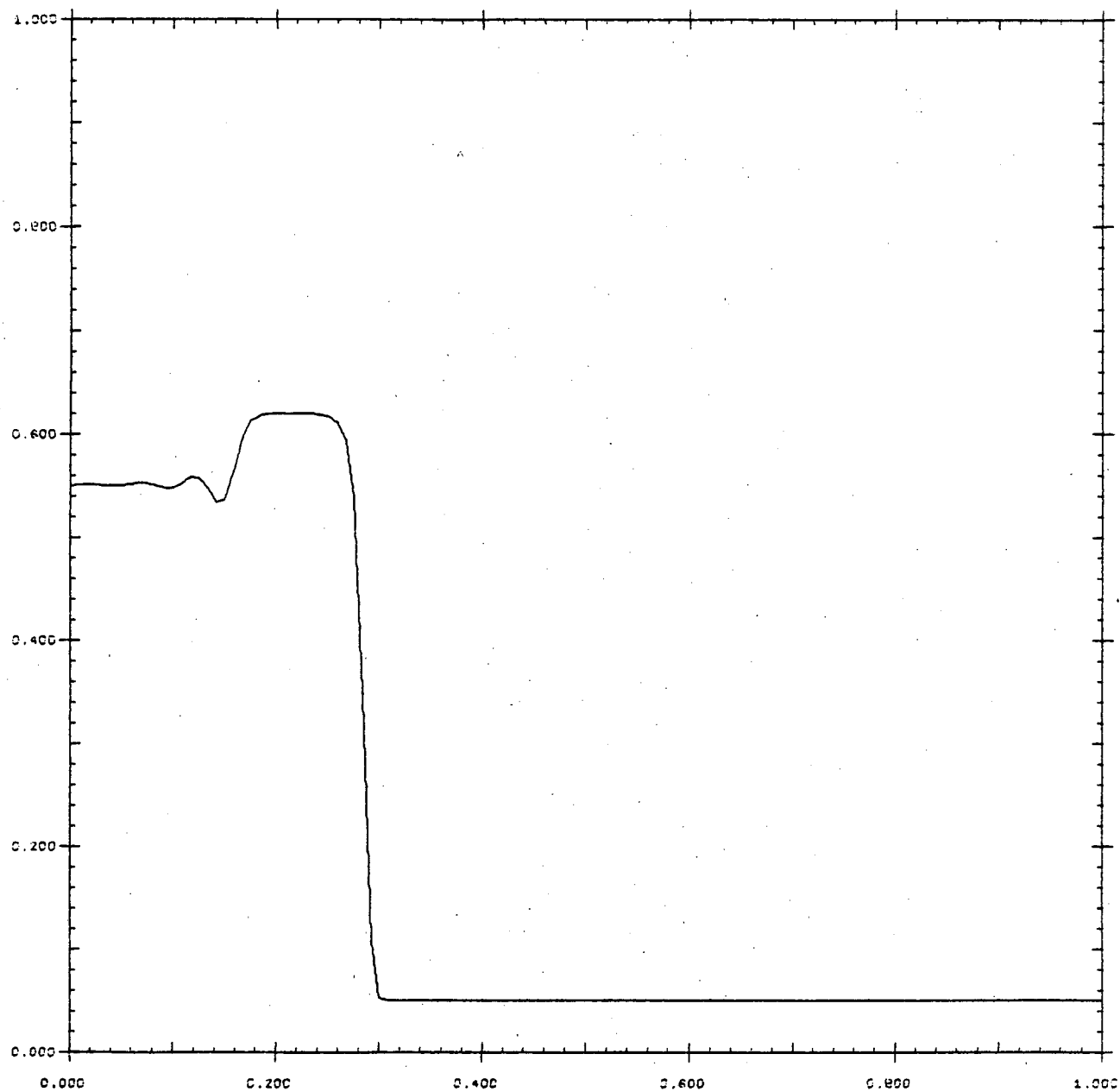


Figure 3a. Shows plot of Lax-Wendroff solution
compressed 120x in direction of x-axis:
50 steps.

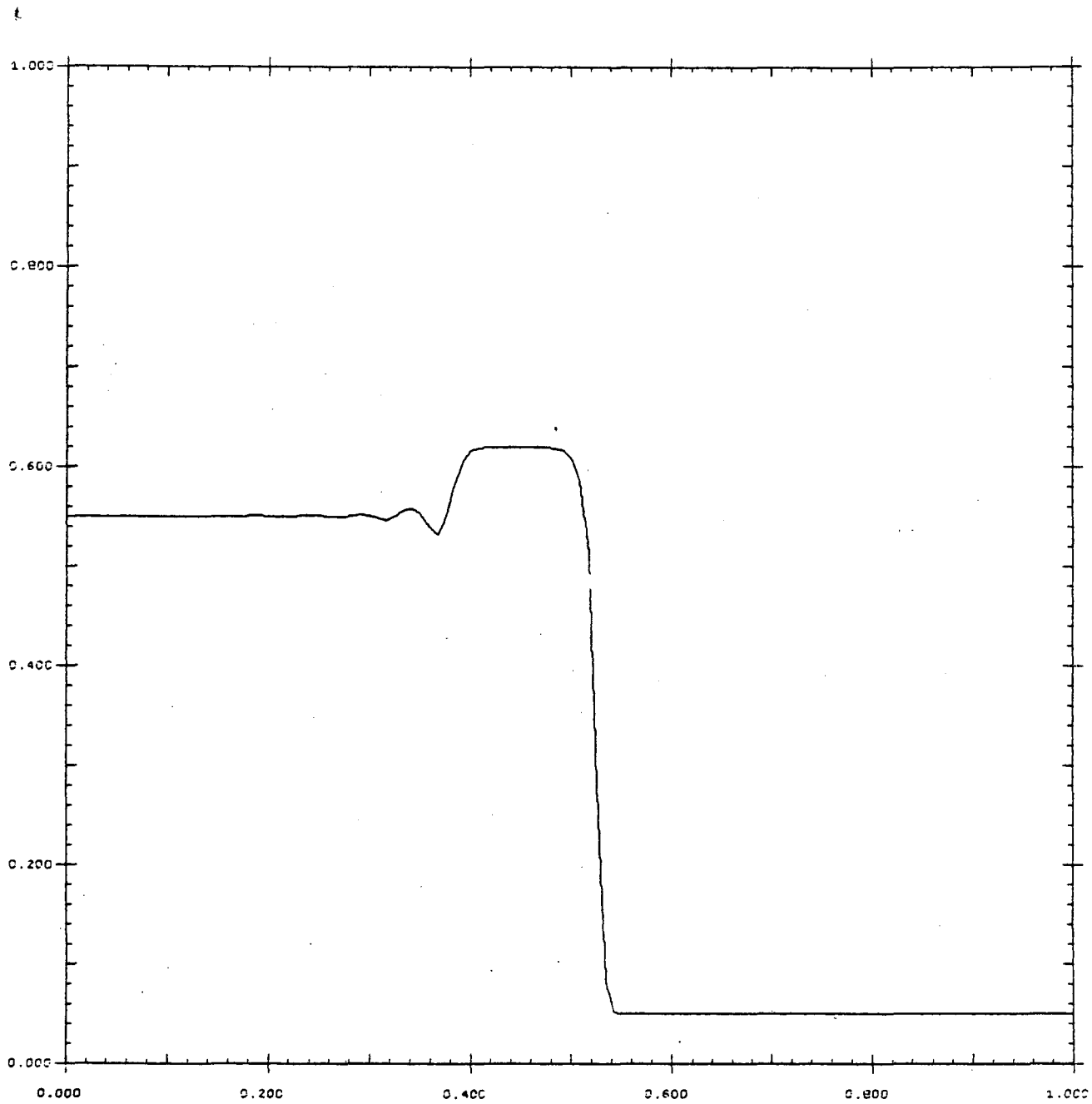


Figure 3b. 100 steps

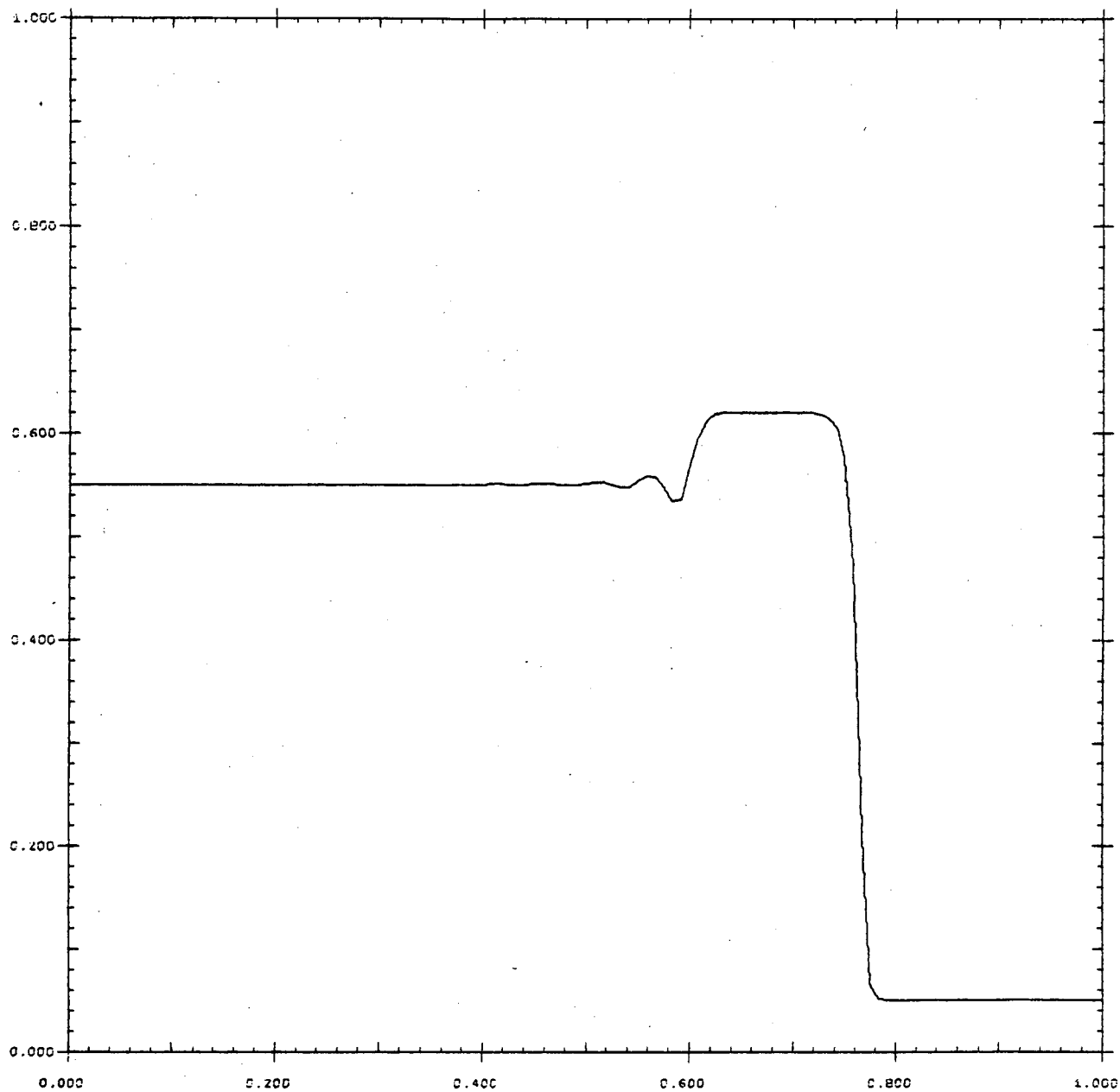


Figure 3c. 150 steps.

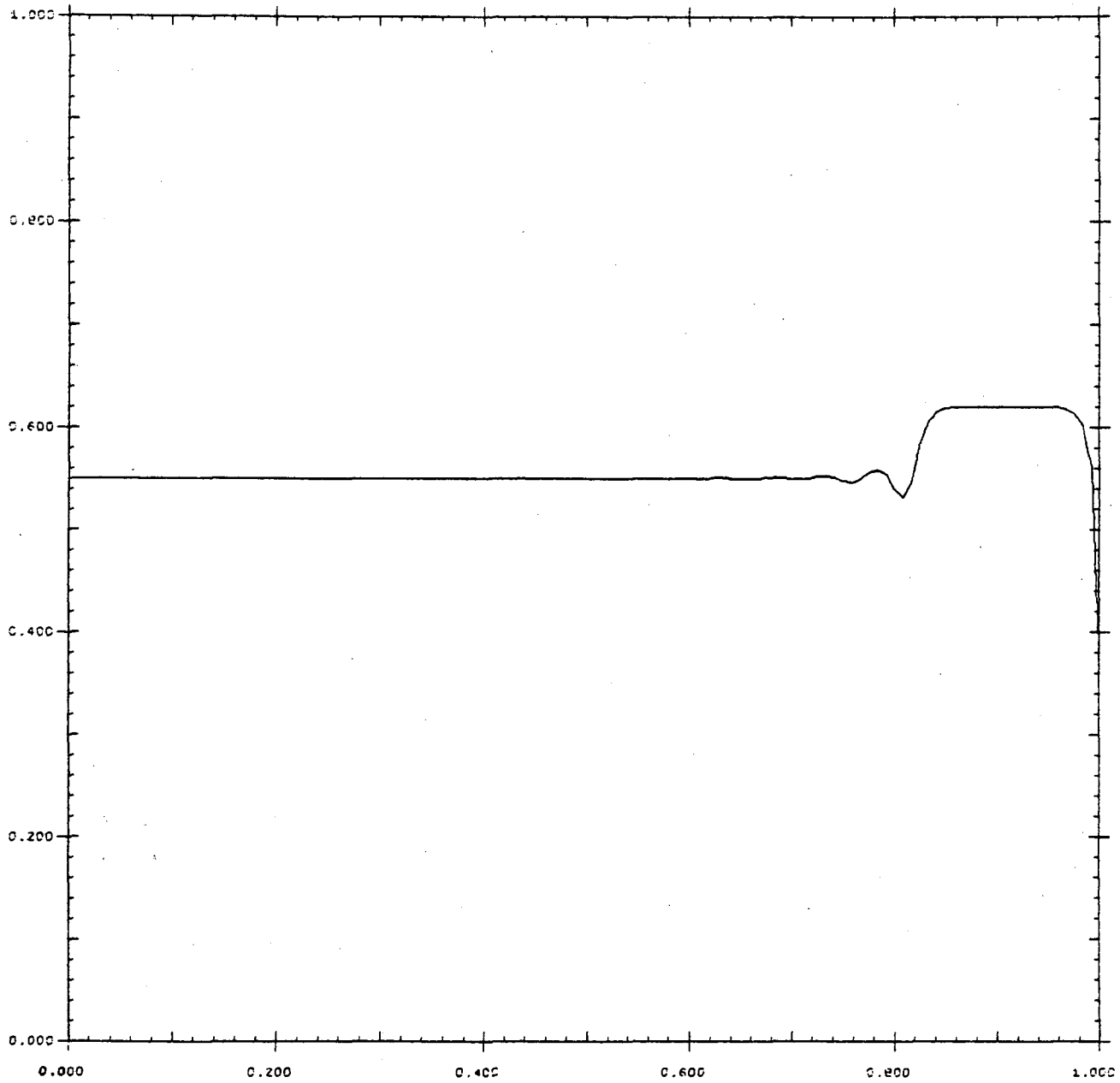


Figure 3d. 200 steps.

[illegible][illegible][illegible][illegible]

0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550
0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550
0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550
0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550
0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550
0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550
0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550
0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550
0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550
0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.549	0.549
0.549	0.548	0.548	0.547	0.546	0.544	0.543	0.540	0.537	0.532	0.524	0.509	0.470

Figure 4

[illegible][illegible][illegible][illegible]

0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550
0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550
0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550
0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550
0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550
0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550
0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550
0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550
0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550
0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550	0.550
0.543	0.540	0.537	0.532	0.524	0.509	0.470	0.259	0.056	0.050	0.050	0.050	0.050

Figure 5

RANDOM CHOICE METHOD BUCKLEY-LEVERETT EQUATION

INITIAL DATA

[illegible]

50 STEPS

[illegible]

100 STEPS

[illegible]

150 STEPS

[illegible]

200 STEPS

[illegible]

Figure 6

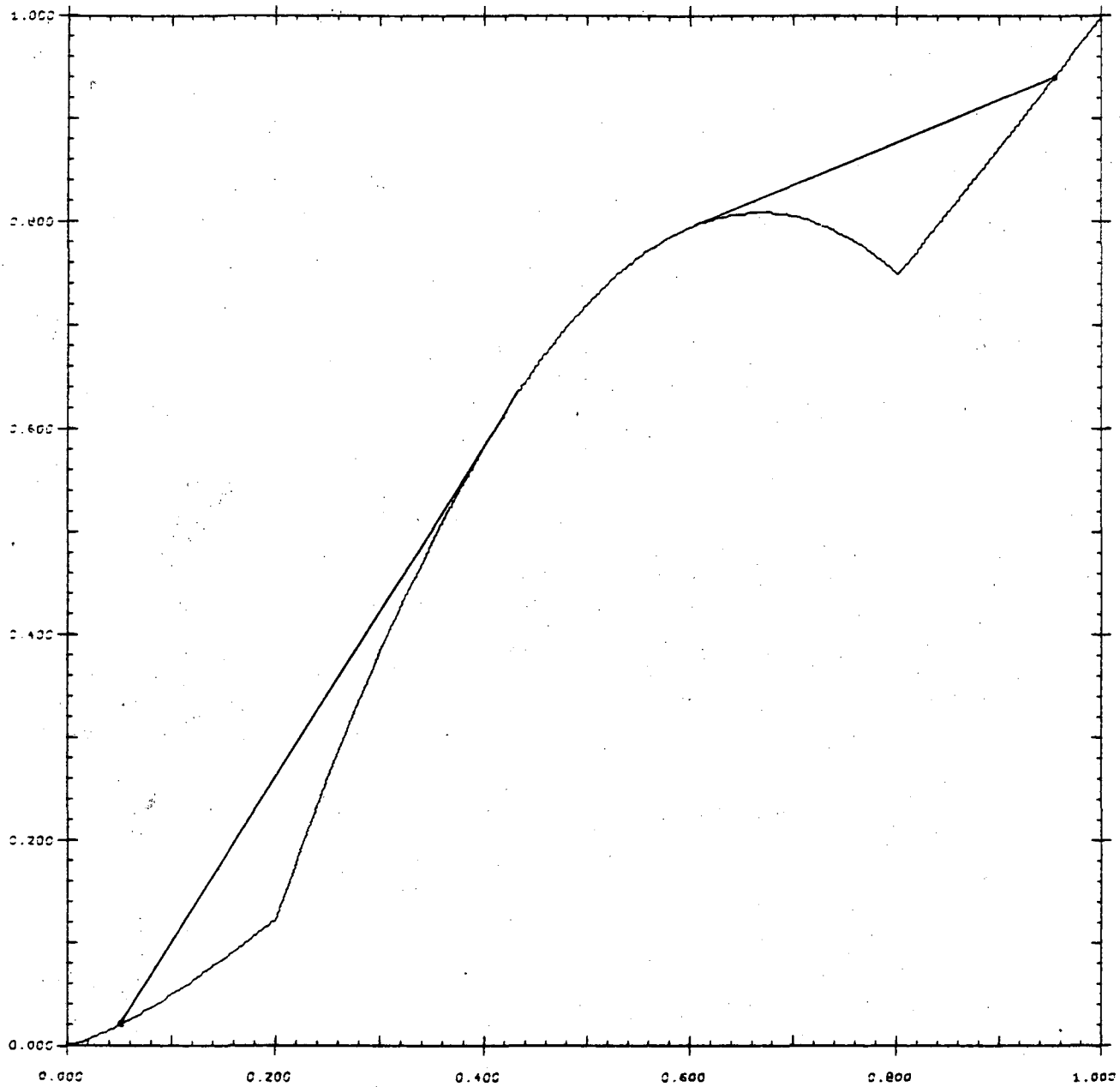


Figure 7. Shows the function $f(u)$ described in text and its convex hull, for $u_R = 0.05$, $u_L = 0.95$.

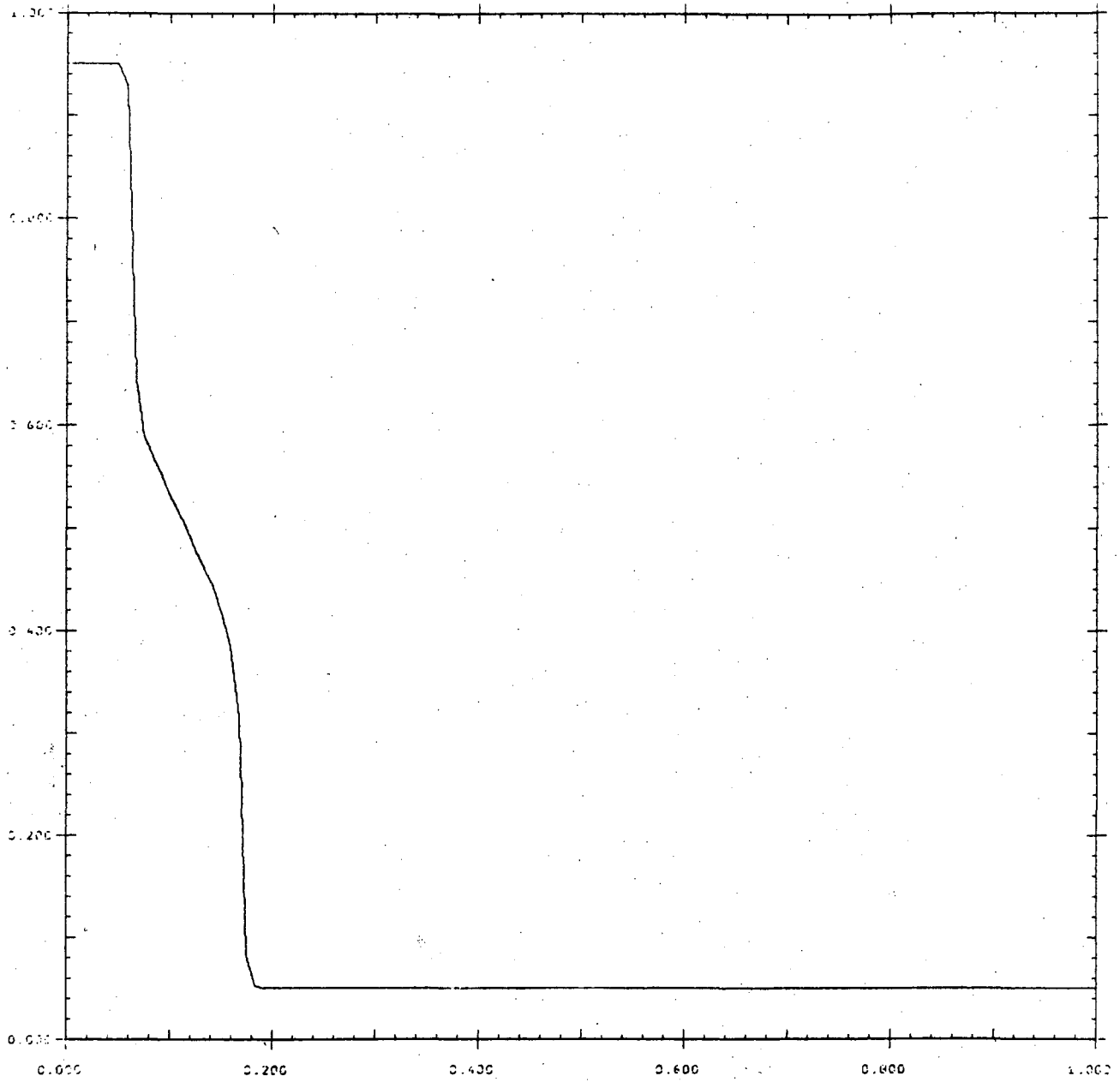


Figure 8a. Shows Godunov scheme with shock on left.

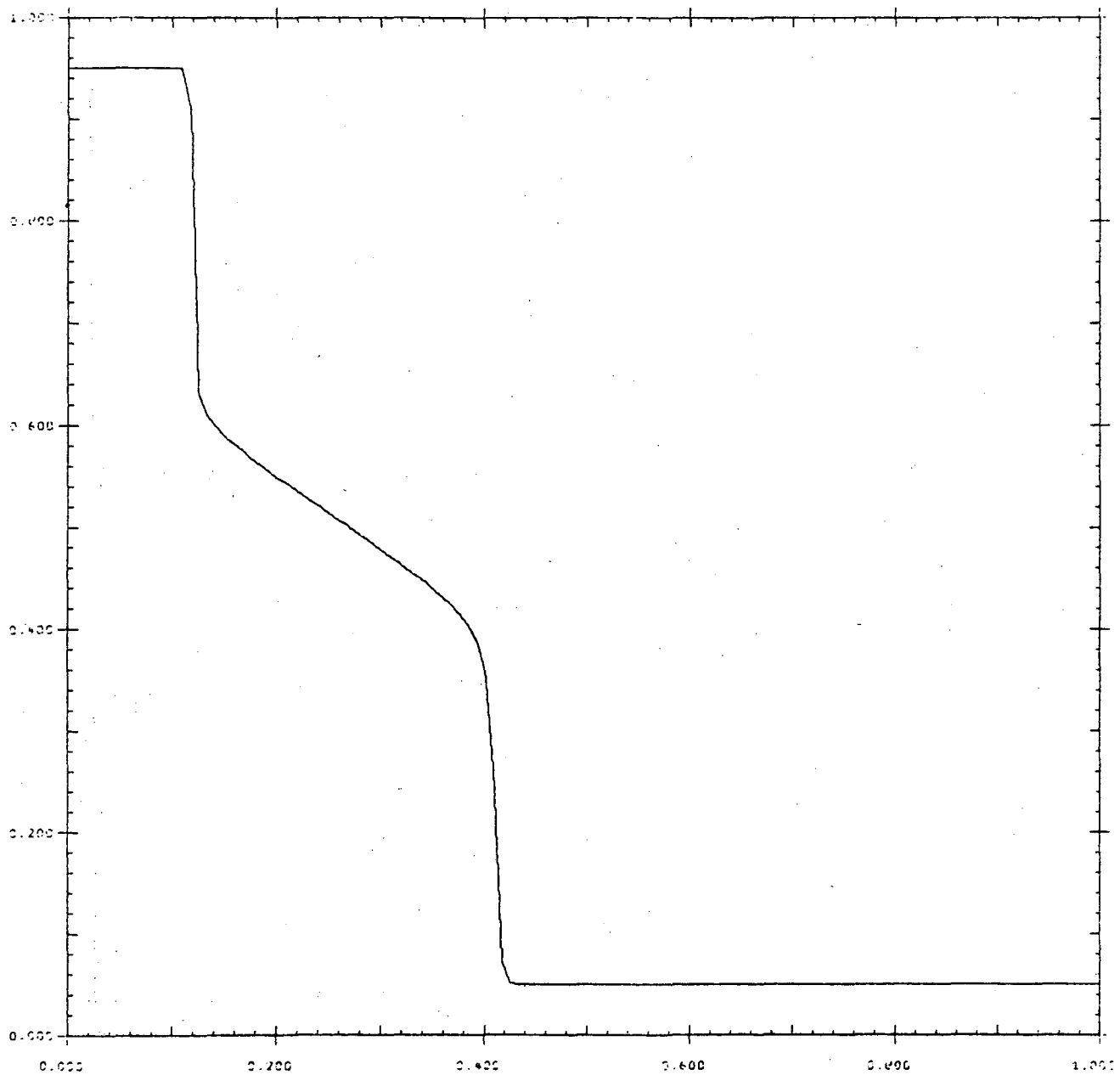


Figure 8b

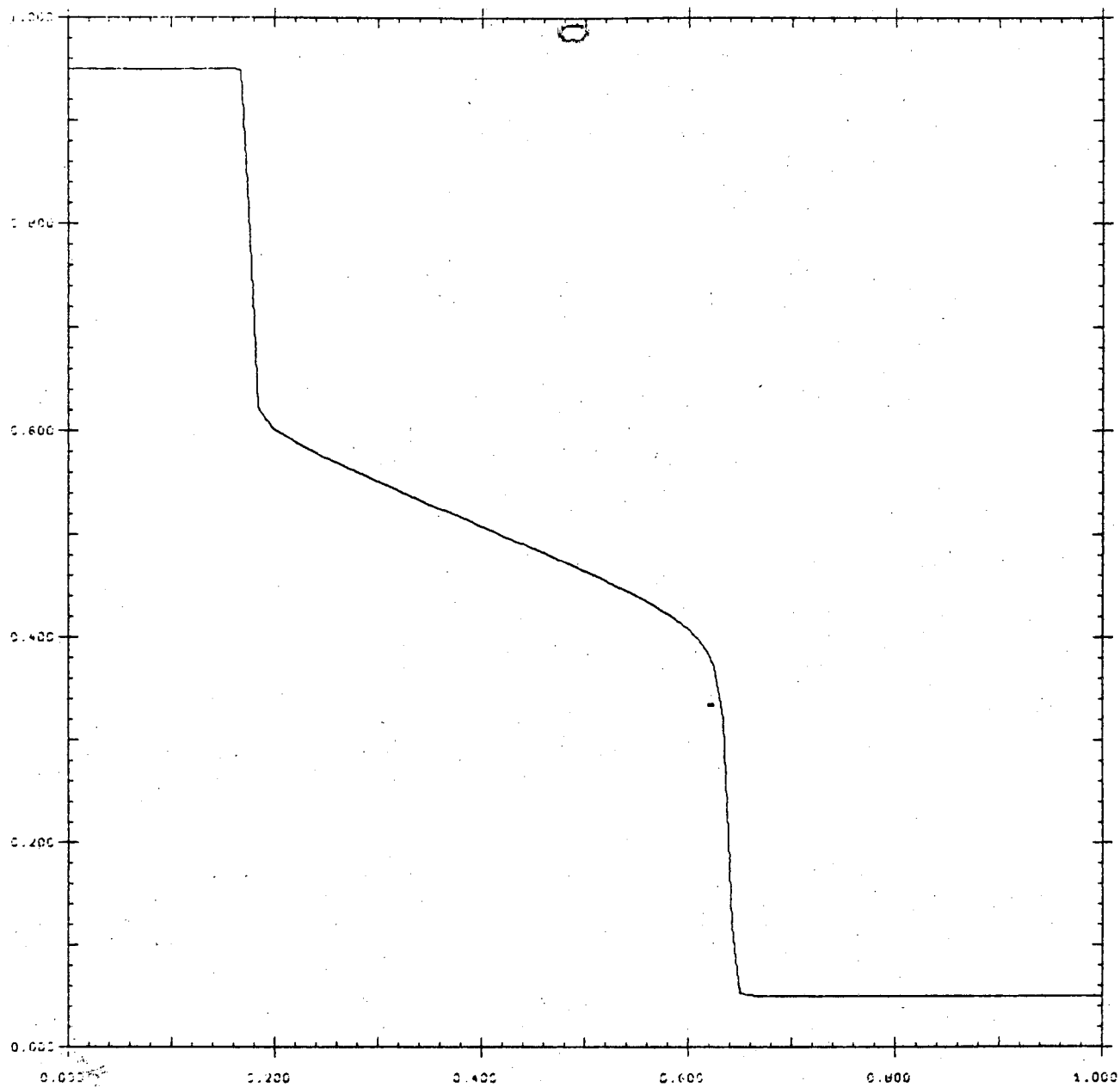


Figure 8c

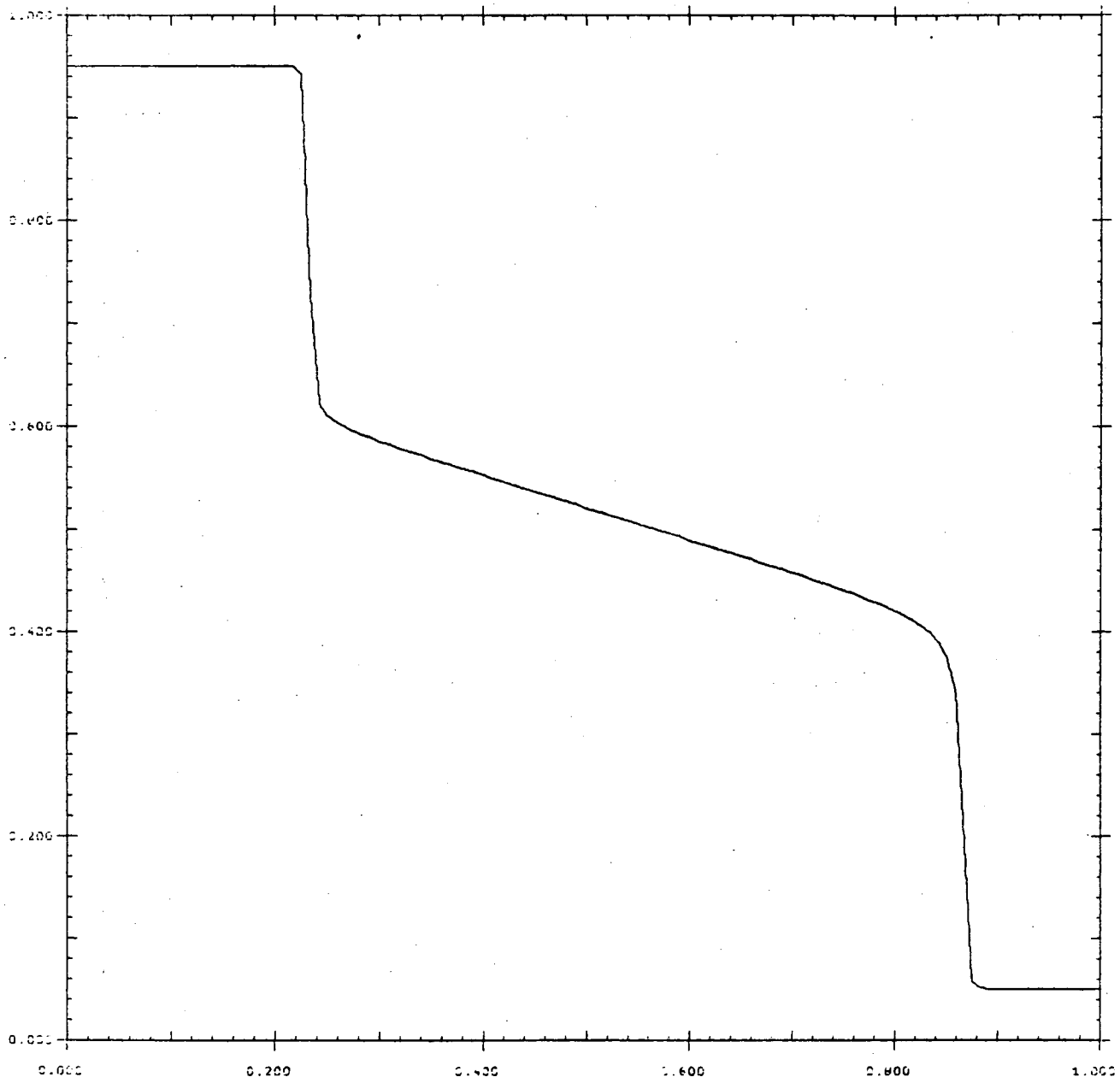


Figure 8d

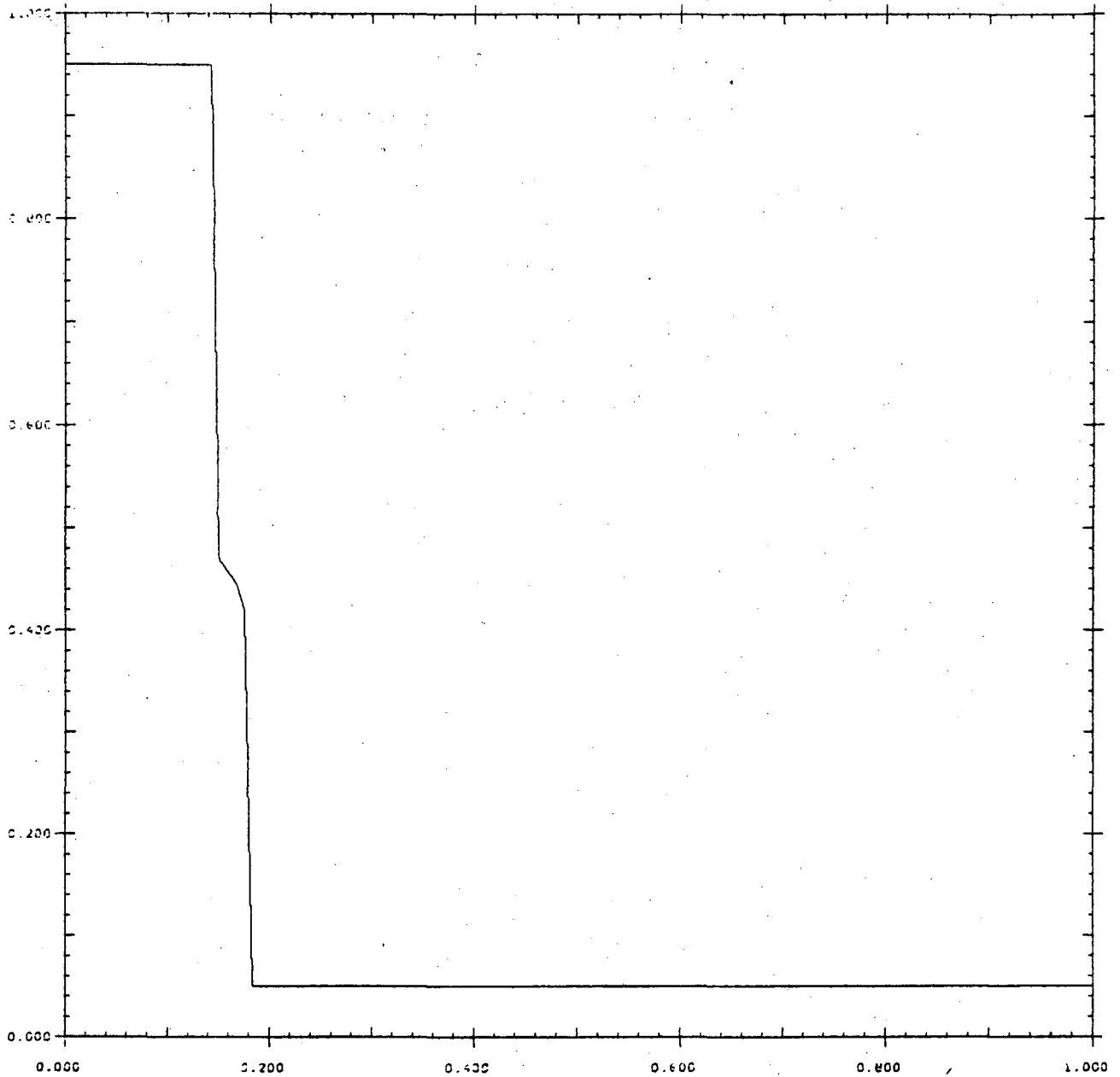


Figure 9a. Shows RCM with 2 sharp progressing shocks.

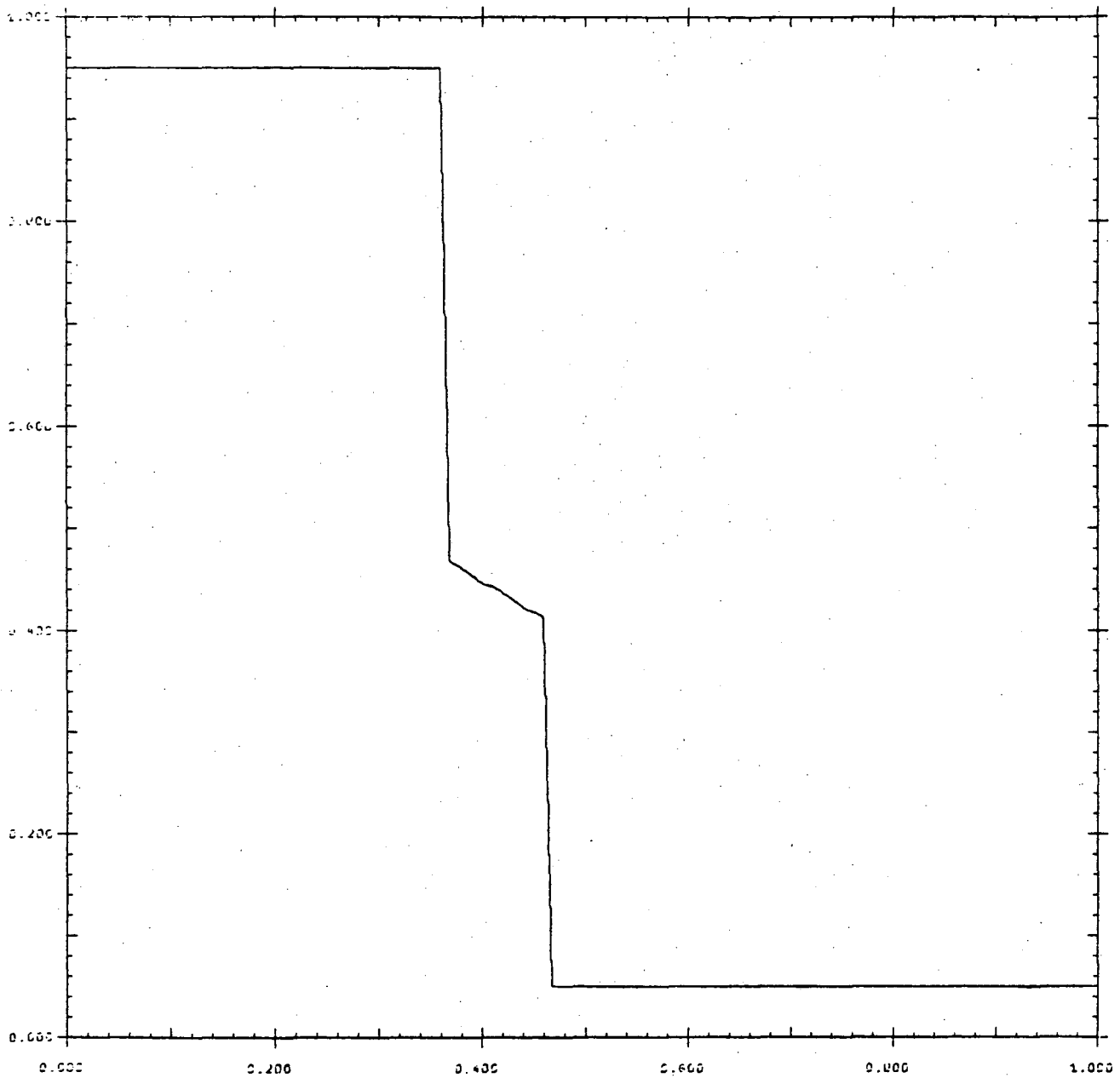


Figure 9b

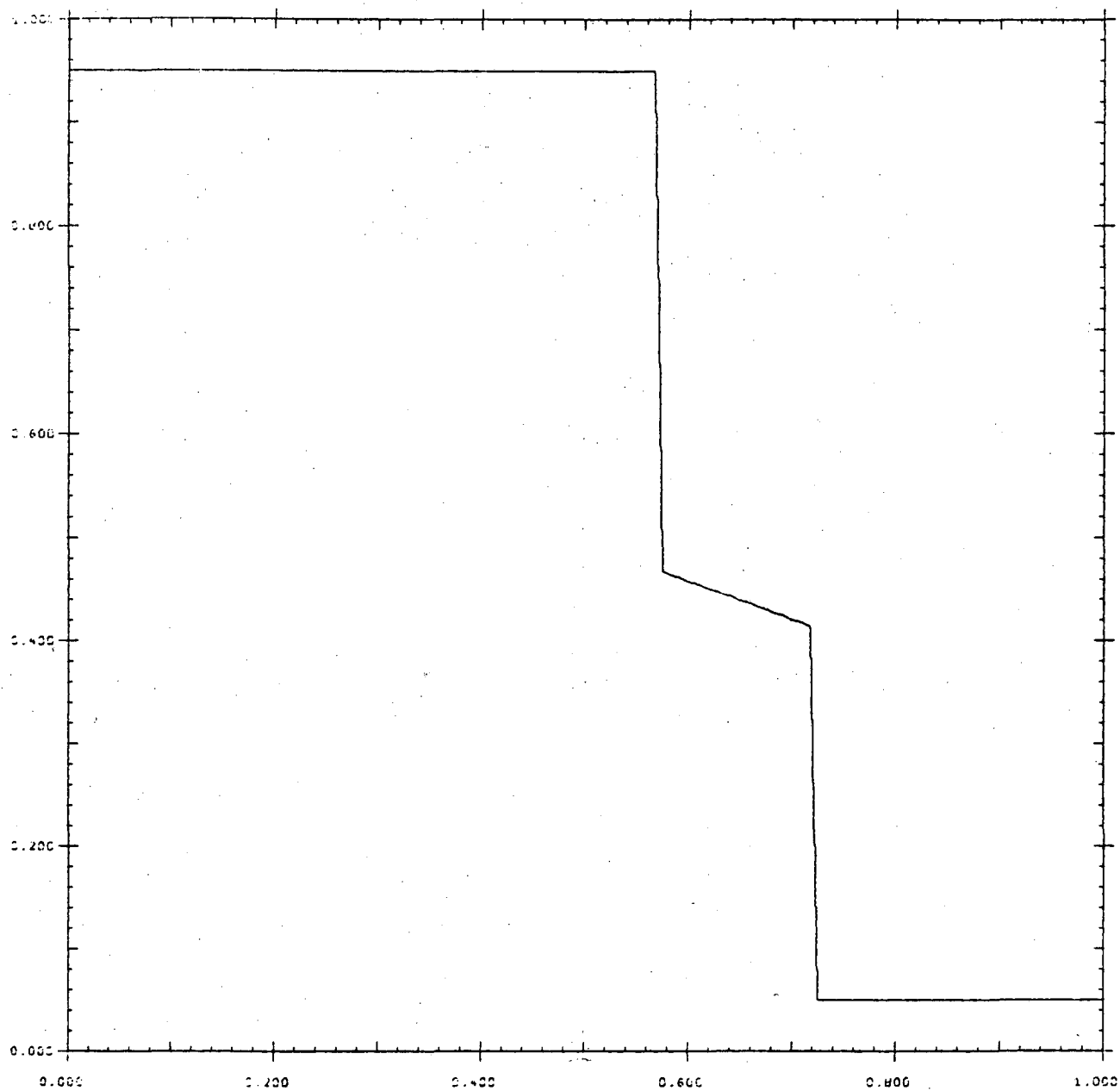


Figure 9c

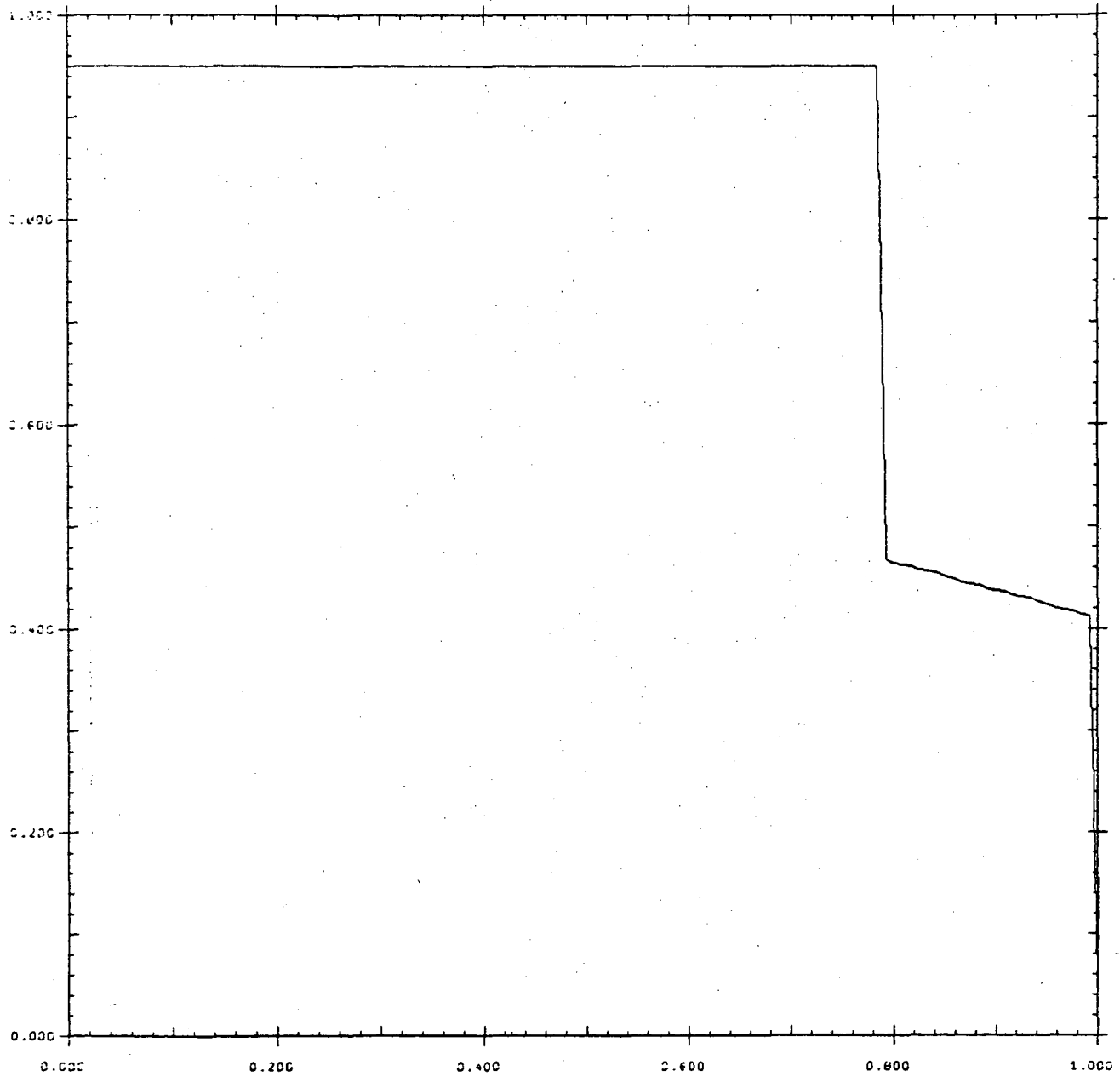


Figure 9d

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