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IN Variant Imbedding,
Particle Interaction and
Conservation Relations
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PREFACE

In this Memorandum the authors present further mathematical results concerning particle-transport processes. Research in the mathematical physics of wave propagation has important implications for a variety of physical situations in such fields as astrophysics and radiation studies.
SUMMARY

In a series of papers, the authors have applied invariant imbedding to provide new analytic and computational approaches to a variety of processes of mathematical physics. We began a detailed analysis of the ordinary and partial differential equations of invariant imbedding, concentrating upon existence and uniqueness of solution, nonnegativity of solution, and convergence of associated difference algorithms as step-size went to zero.

In this paper, we wish to show that for a quite general class of transport processes involving particle-particle interaction, as well as the usual particle-medium interaction, we can obtain difference approximations which exhibit nonnegativity and boundedness in an immediate fashion. Furthermore, a uniform Lipschitz condition is preserved. In subsequent papers the more difficult matters of convergence to the solution of the partial differential equation, and existence of this solution over the entire physical range of the independent variables, will be discussed.
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1. INTRODUCTION

In a series of papers, the technique of invariant imbedding has been applied to provide new analytic and computational approaches to a variety of processes of mathematical physics [1], [2], [3]. In [4], [5], [6], a detailed analysis was begun of the ordinary and partial differential equations of invariant imbedding, concentrating upon existence and uniqueness of solution, nonnegativity of solution, and convergence of associated difference algorithms as step-size went to zero.

In this paper, we wish to show that for a quite general class of transport processes involving particle-particle interaction, as well as the usual particle-medium interaction, we can obtain difference approximations which exhibit nonnegativity and boundedness in an immediate fashion. Furthermore, a uniform Lipschitz condition is preserved. In subsequent papers, we shall discuss the more difficult matters of convergence to the solution of the partial differential equation and existence of this solution over the entire physical range of the independent variables.

2. ANALYTIC AND PHYSICAL PRELIMINARIES

When interaction occurs, the expected fluxes in the transport process do not depend linearly upon the
incident fluxes. To apply invariant imbedding techniques we must regard the reflection, transmission, and loss functions as functions of both the length of the rod and the incident intensities. We let

\[ r_i(x,y) = \text{the expected flux of particles in state } i \text{ reflected from a rod of length } x \text{ when the incident flux at } x \text{ has intensity } y. \]

Here, the incident intensity \( y \) is an \( N \)-dimensional vector whose \( j \)-th component \( y_j \) is the intensity of incident flux in state \( j \). For convenience we also introduce the column vector \( r(x,y) \) with components \( r_i(x,y) \) \( (i = 1,2,...,N) \).

The transmission and loss vector functions, \( t(x,y) \) and \( l(x,y) \), are defined similarly. We let

\[ t_i(x,y) = \text{the expected flux of particles in state } i \text{ transmitted through a rod of length } x \text{ when the incident flux at } x \text{ has intensity } y; \]

\[ l_i(x,y) = \text{the expected flux of particles in state } i \text{ absorbed or annihilated within a rod of length } x \text{ when the incident flux at } x \text{ has intensity } y. \]
To obtain differential equations for these functions, we consider a discrete approximation to the process in which the rod is divided up into small segments, each of length $\Delta$. In setting up the discrete approximation, we shall often ignore terms of higher order than $\Delta$ since the partial differential equations obtained by letting $\Delta$ approach 0 will not depend upon higher order terms. This still leaves considerable freedom in the choice of the discrete approximation. We take advantage of this freedom by selecting a discrete approximation which preserves two important features of the physical problem—nonnegativity and conservation of matter. The difference equations will be chosen so that the components of $r(x,y)$, $t(x,y)$, and $l(x,y)$ are all obviously nonnegative and so that

$$
(2.3) \quad \sum_{i=1}^{N} (r_i(x,y) + t_i(x,y) + l_i(x,y)) = \sum_{i=1}^{N} y_i.
$$

We now consider what happens in the segment $[x, x + \Delta]$. When a flux of $u_j$ particles in state $j$ enters the segment at one end and a flux of $v_k$ particles in state $k$ enters at the other end, then the following effects occur:

(a) The expected number of particles from the $u_j$-stream absorbed by the medium is $f_{jj}(x)u_j\Delta + O(\Delta^2)$, and the expected number absorbed from the $v_k$-stream is $f_{kk}(x)v_k\Delta + O(\Delta^2)$. 
(b) The expected number of particles from the 
\(u_j\)-flux back-scattered in state \(i\) is \(b_{ij}(x)u_j \Delta + O(\Delta^2)\),
and the expected number from the \(v_k\)-flux back-scattered
in state \(i\) is \(b_{ik}(x)v_k \Delta + O(\Delta^2)\).

c) The expected number from the \(u_j\)-stream transmitted in state \(i\) (\(i \neq j\)) is \(d_{ij}(x)u_j \Delta + O(\Delta^2)\), and the expected number from the \(v_k\)-flux transmitted in state \(i\) (\(i \neq k\)) is \(d_{ik}(x)v_k \Delta + O(\Delta^2)\).

In addition to these effects, which would occur in a
no-interaction model, we introduce collision effects.
Let \(u\) denote the column vector with \(j\)-th component \(u_j\)
for \(j = 1, 2, \ldots, N\), and let \(v\) denote the vector with
components \(v_1, v_2, \ldots, v_N\). Then:

d) The expected number of articles from the \(u_j\)-stream annihilated due to interactions with the opposing streams with intensities given by the vector \(v\) is

\[
(2.4) \quad u_j \varphi_j(u_j, v, x) \Delta + O(\Delta^2) = u_j \left[ 1 - e^{-\Delta \varphi_j(u_j, v, x)} \right] + O(\Delta^2).
\]

Similarly, the expected number annihilated from the \(v_k\)-stream due to interactions with the opposing streams represented by the vector \(u\) is

\[
(2.5) \quad v_k \left[ 1 - e^{-\Delta \varphi_k(v_k, u, x)} \right] + O(\Delta^2).
\]
The functions $\varphi_j$ are constrained by the conditions

\begin{equation}
\varphi_j(u_j,v,x) \geq 0, \quad \varphi_j(u_j,0,x) = 0, \\
\lim_{x \to 0} u_j \varphi_j(u_j,v,x) = 0.
\end{equation}

In setting up the difference approximation, we have used the exponentials to obtain terms which are obviously nonnegative and uniformly bounded if the conditions of (2.6) hold.

In the following discussion we shall usually suppress the $x$-dependence of $f_{jj}(x)$, $b_{ij}(x)$, etc. We assume that

\begin{equation}
b_{ij} \geq 0, \quad d_{ij} \geq 0 \quad (i \neq j), \quad f_{jj} \geq 0;
\end{equation}

and we define $d_{jj}$ by the equation

\begin{equation}
d_{jj} = - \left[ \sum_{i=1}^{N} b_{ij} + \sum_{i=1}^{N} d_{ij} + f_{jj} \right] \quad (j = 1,2,...,N),
\end{equation}

which implies that $d_{jj} \leq 0$. If we introduce the matrices

\begin{equation}
D(x) = (d_{ij}(x)), \quad B(x) = (b_{ij}(x)), \quad F(x) = (f_{jj}(x)\delta_{ij}),
\end{equation}

\begin{equation}
M = \begin{pmatrix}
1 & 1 & \cdots & 1 \\
0 & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & 0
\end{pmatrix},
\end{equation}

then from (2.8) we obtain the relation
\[(2.10) \quad M(B + D + F) = 0.\]

It is also convenient to introduce the matrix
\[(2.11) \quad \phi(u,v,x) = (\varphi_i(u_i,v,x)\delta_{ij}).\]

To derive the difference equations for our discrete approximation, we introduce the auxiliary vector function \(v(x,y)\) where
\[(2.12) \quad v_i(x,y) = \text{the expected flux in state } i \text{ moving to the left at } x \text{ due to an incident flux at } x + \Delta \text{ of intensity } y.\]

To terms of order \(\Delta\), the flux \(v(x,y)\) arises from forward scattering of \(y\) diminished by absorption and annihilation, and from back scattering of the flux incident at \(x\) which is moving to the right. The flux at \(x\) moving to the right is \(r(x,v(x,y))\). Hence, to terms of order \(\Delta\), we obtain
\[(2.13) \quad v(x,y) = (I + \Delta D)e^{-\Delta \phi(y,r(x,v(x,y)))}y + \Delta Br(x,v(x,y)),\]

an implicit equation for \(v\). Since this implicit equation seems to be somewhat difficult to handle, we shall replace \(\phi(y,r(x,v(x,y)))\) by \(\phi(y,r(x,y))\). If \(r(x,v)\) satisfies a uniform Lipschitz condition and \(v(x,y) = y + O(\Delta)\), this replacement will only affect terms of higher order.
The reflected flux at \( x + \Delta \) arises from fluxes of intensity \( y \) and \( r(x,v(x,y)) \) incident upon the segment from \( x \) to \( x + \Delta \). Hence, to terms of order \( \Delta \) we obtain

\[
(2.14) \quad r(x + \Delta, y) = \Delta By \\
+ (I + \Delta D)e^{-\Delta \Phi(r(x,y),y)} r(x,v(x,y)),
\]

where the two terms represent backward and forward scattering, respectively. Similarly we obtain

\[
(2.15) \quad t(x + \Delta, y) = t(x,v(x,y)).
\]

In calculating the loss functions, we break it up into losses occurring in the segment \([0,x]\) and in the segment \([x,x + \Delta]\). In the latter we must consider losses due to absorption from both the \( y \)-flux and the \( r(x,v(x,y)) \)-flux, and losses due to annihilation of particles from both fluxes. We obtain

\[
(2.16) \quad l(x + \Delta, y) = l(x,v(x,y)) \\
+ \Delta FY + \Delta Fr(x,v(x,y)) \\
+ (I + \Delta D)(I - e^{-\Delta \Phi(r(x,y),y)}) r(x,v(x,y)) \\
+ (I + \Delta D)(I - e^{-\Delta \Phi(y,r(x,y))}) y.
\]

3. THE DEFINING EQUATIONS

In the following discussion we shall proceed rigorously, using the difference equations obtained above as
our starting point. The fundamental vector equations for 
\[ x = 0, \Delta, 2\Delta, 3\Delta, \ldots, \quad y \geq 0, \]
are thus the difference equations

\[ r(x + \Delta, y) = ABy + (I + AD)e^{-\Delta\Phi}(r(x, y), y)r(x, v(x, y)), \]
\[ t(x + \Delta, y) = t(x, v(x, y)), \]
\[ l(x + \Delta, y) = l(x, v(x, y)) + \Delta Fy + \Delta Fr(x, v(x, y)) \]
\[ + [I + AD][1 - e^{-\Delta\Phi}(y, r(x, y))]y \]
\[ + [I + AD][1 - e^{-\Delta\Phi}(r(x, y), y)]r(x, v(x, y)), \]
and the implicit equation

\[ v(x, y) = (I + AD)e^{-\Delta\Phi}(y, r(x, y)) + ABr(x, v(x, y)). \]

For intermediate values of \( x \) we shall assume that the functions \( r(x, y), t(x, y), \) and \( l(x, y) \) are defined by linear interpolation.

For the problem we have discussed, we have the following initial conditions corresponding to a rod of length 0:

\[ r(0, y) = 0, \quad t(0, y) = y, \quad l(0, y) = 0; \]

but to allow comparison with other initial value problems for partial differential equations, we shall allow the more general situation in which

\[ r(0, y) = g(y), \quad t(0, y) = y, \quad l(0, y) = 0. \]
In our problem this situation would arise if there were a source at 0 or additional material to the left of 0. We shall assume that \( g(y) \geq 0 \) and satisfies a Lipschitz condition

\[
\|g(y) - g(y')\| \leq L_0 \|y - y'\|,
\]

where \( L_0 \) is a positive constant.

The scheme (3.1) and (3.2) is not immediately usable for numerical purposes because (3.2) is an implicit equation for \( v \). For numerical purposes we would expect to solve (3.2) by iteration, starting with the initial approximation \((I + AD)e^{-\Delta t}(y, r(x,y))y\) for \( v \). Observe that if the iterations converge to a solution of (3.2), then because of (2.7) all components of the limit vector \( v(x,y) \) will be nonnegative provided \( \Delta \) is sufficiently small so that \( I + \Delta D \) has nonnegative elements. Similarly, nonnegativity of \( r, t, \) and \( l \) is preserved.

4. LIMITING DIFFERENTIAL EQUATIONS

From the foregoing equations, we obtain formally a set of nonlinear partial differential equations for \( r, t, \) and \( l \) by passing to the limit in \( \Delta \). Introduce the three Jacobian matrices

\[
\frac{\partial}{\partial y} = \sum_{i=1}^{N} |y_i|, \quad \|B\| = \sum_{i,j=1}^{N} |b_{ij}|.
\]
Using (3.2) in conjunction with (3.1), we readily obtain the nonlinear partial differential equations

\begin{align}
(4.2) \quad & r_x - R_y [D_y + Br - \phi(y,r)y] = By + Dr - \phi(r,y)y, \\
& t_x - T_y [D_y + Br - \phi(y,r)y] = 0, \\
& \ell_x - L_y [D_y + Br - \phi(y,r)y] = Fy + Fr + \phi(y,r)y + \phi(r,y)r.
\end{align}

From (3.3) we obtain the initial conditions

\begin{align}
(4.3) \quad & r(0,y) = g(y), \quad t(0,y) = y, \quad \ell(0,y) = 0.
\end{align}

5. CONSERVATION FOR THE DISCRETE APPROXIMATION

For the considerations of this section it is convenient to replace the initial conditions (3.3) by the conditions

\begin{align}
(5.1) \quad & r(0,y) = z, \quad t(0,y) = y, \quad \ell(0,y) = 0,
\end{align}

where \( z \) is an arbitrary nonnegative \( N \)-dimensional vector which may depend upon \( y \). The discrete approximation given by (3.1) and (3.2) was chosen so that the following conservation relation would hold:
This states that the total reflected flux, transmitted flux, and dissipation due to absorption and annihilation must equal the total input at the ends of the rod—what goes in must equal what goes out.

We shall take up the question of existence of solutions of (3.1) and (3.2) later. In this section, assuming the existence of solutions of (3.1) and (3.2), we prove by induction that the conservation relation (5.2) holds for \( x = 0, \Delta, 2\Delta, 3\Delta, \ldots \). First, for \( x = 0 \) the conservation relation follows immediately from (5.1). As our induction hypothesis, we assume that (5.2) holds for \( x \) for all input vectors \( y \) and \( z \), and we then show that it holds for \( x + \Delta \). Abbreviating \( r(x,y) \) by \( r \) and \( v(x,y) \) by \( v \) and making use of (2.10), we have

\[
\begin{align*}
(5.3) \quad M[r(x+\Delta,y) + t(x+\Delta,y) + l(x+\Delta,y)] &= M[y + z] - \Delta MB_y - \Delta MB_r(x,v) + M[I+\Delta D]y - M[I+\Delta D]e^{-\Delta \Phi(y,r)}y
\end{align*}
\]
which completes the proof by induction.

6. EXISTENCE OF SOLUTIONS FOR DISCRETE APPROXIMATION

We shall now prove the existence of a solution of (3.1) — (3.2) satisfying the initial conditions (3.3) for a small \( x \) interval provided the step size \( \triangle \) is sufficiently small. At the same time we shall show that \( r(x,y) \) satisfies a Lipschitz condition with respect to \( y \) which is uniform in \( \triangle \). In addition to the assumptions already made concerning \( B(x), D(x), F(x), \Phi(u,v,x), \) and \( g(y) \), we assume that \( B(x) \) and \( D(x) \) are uniformly bounded and \( \Phi(u,v,x) \) satisfies uniform Lipschitz conditions with respect to \( u \) and \( v \).

The proof will be carried out inductively for a region of the form

\[(6.1) \quad y \geq 0, \quad \gamma y \leq c e^{-\gamma x} - c_1,\]

where \( \gamma \) is any positive constant for which

\[(6.2) \quad \gamma > \|B\| + \|D\|,\]

\( c \) is an arbitrary positive constant, and \( c_1 > z \), where \( z = g(y) \) is the input flux vector at 0. We show that the system (3.1) — (3.2) has a solution for \( 0 \leq x \leq x^* \) provided \( 0 < \triangle \leq \delta \), where \( x^* \) and \( \delta \) depend upon the constants \( c, \gamma, \) and \( c_1 \) as well as upon \( B(x), D(x), \Phi(u,v,x), \) and \( g(y) \).
As our induction hypothesis we assume (a) that for \( y \) and \( y' \) satisfying (6.1), we have

\[
(6.3) \quad \|r(x,y) - r(x,y')\| \leq L(x)\|y - y'\|,
\]

where \( L(x) \) is a certain function of \( x \) to be specified below; (b) that the conservation relation

\[
(6.4) \quad M[r(x,y) + t(x,y) + l(x,y)] = M(y + z)
\]

holds, and (c) that \( r(x,y) \geq 0 \). Under these assumptions we prove that for \( 0 < \Delta \leq \delta, \ 0 \leq x \leq x^* \) the equation (3.2) has a nonnegative solution \( v(x,y) \) for \( y \geq 0, \ |y| \leq ce^{-\gamma(x+\Delta)} - c_1 \). It will then follow immediately that for

\[
(6.5) \quad y \geq 0, \ |y| \leq ce^{-\gamma(x+\Delta)} - c_1,
\]

the vectors \( r(x + \Delta, y), t(x + \Delta, y), \) and \( l(x + \Delta, y) \) determined by (3.1) are nonnegative and, by the proof given previously, satisfy \( M[r(x+\Delta,y) + t(x+\Delta,y) + l(x+\Delta,y)] = M(y + z) \). We then show that for \( y \) and \( y' \) in the region (6.1), we have

\[
(6.6) \quad \|r(x + \Delta, y) - r(x + \Delta, y')\| \leq L(x + \Delta)\|y - y'\|,
\]

thus completing the inductive step from \( x \) to \( x + \Delta \).

We obtain a solution of (3.2) by iteration, starting with the vector \( v_0 = (I + \Delta D)e^{-\Delta \Phi} y \) and defining the vectors \( v_1, v_2, \ldots \) recursively by the equation
\[ v_{n+1} = v_0 + \Delta B r(x,v_n). \]

Because all elements of the matrix \( B \) are nonnegative, each component of \( v_n \) increases monotonically with \( n \). Thus to prove that the sequence \( v_0, v_1, v_2, \ldots \) converges, it is sufficient to show that the sequence is uniformly bounded. By (6.4) we have

\[ \|v_{n+1}\| \leq \|v_0\| + \|\Delta B\| (\|v_n\| + \|z\|); \]

hence

\[ \|v_{n+1}\| + c_1 \leq \|v_0\| + c_1 + \|\Delta B\| (\|v_n\| + c_1), \]

and by induction

\[ \|v_{n+1}\| + c_1 \leq (\|v_0\| + c_1) \cdot (1 + \|\Delta B\| + \|\Delta B\|^2 + \cdots + \|\Delta B\|^n). \]

Thus if \( \|\Delta B\| < 1 \), the sequence converges and the limit function \( v(x,y) = \lim_{n \to \infty} v_n \) satisfies

\[ \|v(x,y)\| + c_1 \leq \frac{\|v_0\| + c_1}{1 - \|\Delta B\|} \leq \frac{1 + \|\Delta B\|}{1 - \|\Delta B\|}(\|y\| + c_1) \]

\[ < (1 + \gamma \Delta)(\|y\| + c_1) \]

\[ < e^{\gamma \Delta}(\|y\| + c_1), \]

provided \( \Delta \) is sufficiently small. Note that \( v(x,y) \geq 0 \) and that if \( y \) satisfies (6.1), then

\[ \|v(x,y)\| \leq c e^{-\gamma(x+\Delta)} - c_1. \]

Because \( r(x,v) \) is a
continuous function of $v$ in this region, it follows that the limit function $v(x,y)$ satisfies the equation (3.2).

To establish that $r(x + \Delta, y)$ satisfies a Lipschitz condition, we first prove that $v(x,y)$ satisfies a Lipschitz condition for $y$ and $y'$ in the region (6.5). We have

\begin{equation}
(6.11) \quad v(x,y) = y + \Delta e^{-\Delta e^{\phi}(y,r(x,y))}y + (e^{-\Delta e^{\phi}(y,r(x,y))} - I)y + \Delta Br(x,v(x,y)).
\end{equation}

It is easily seen that if $L(x) \geq L_0$, there is a positive constant $c_2$ such that

\begin{equation}
(6.12) \quad \Delta e^{-\Delta e^{\phi}(y,r(x,y))}y - \Delta e^{-\Delta e^{\phi}(y',r(x,y'))}y' \leq c_2 L(x) \Delta y - y',
\end{equation}

\begin{equation}
\| (e^{-\Delta e^{\phi}(y,r(x,y))} - I)y - (e^{-\Delta e^{\phi}(y',r(x,y'))} - I)y' \| \leq c_2 L(x) \Delta y - y'.
\end{equation}

If $y$ and $y'$ satisfy (6.1), then by (6.10) we have

\begin{equation}
(6.13) \quad \| v(x,y) \| \leq ce^{-\gamma x} - c_1, \quad \| v(x,y') \| \leq ce^{-\gamma x} - c_1.
\end{equation}

Hence,
\[(6.14) \quad \|v(x, y) - v(x, y')\| \leq \|y - y'\| + 2c_2\Delta L(x)\|y - y'\| \\
+ \Delta \|B\| \|r(x, v(x, y)) - r(x, v(x, y'))\| \\
\leq \|y - y'\|(1 + 2c_2\Delta L(x)) \\
+ \Delta \|B\| L(x)\|v(x, y) - v(x, y')\|,
\]

and consequently,

\[(6.15) \quad \|v(x, y) - v(x, y')\| \leq \frac{1 + 2c_2\Delta L(x)}{1 - \Delta \|B\| L(x)} \|y - y'\| \\
< (1 + c_3\Delta L(x))\|y - y'\|
\]

if \(\Delta \|B\| L(x) < 1/2\), where we can let \(c_3 = 2\|B\| + 4c_2\).

We have

\[(6.16) \quad r(x + \Delta, y) = \Delta y + r(x, v(x, y)) \\
+ \Delta e^{-\Delta \phi(r(x, y), y)} r(x, v(x, y)) \\
+ (e^{-\Delta \phi(r(x, y), y)} - 1) r(x, v(x, y)).
\]

For \(y\) and \(y'\) satisfying (6.1), using (6.15) we obtain the estimates
(6.17)  \[ \| \Delta e^{-\Delta \phi (r(x,y),y)} r(x,v(x,y)) - \Delta e^{-\Delta \phi (r(x,y'),y') r(x,v(x,y'))} \| \]

\[ \leq c_4 \Delta L(x) (1 + c_3 \Delta L(x)) \| y - y' \|, \]

\[ \| (e^{-\Delta \phi (r(x,y),y)} - 1) r(x,v(x,y)) - (e^{-\Delta \phi (r(x,y'),y')} - 1) r(x,v(x,y')) \| \]

\[ \leq c_4 \Delta L(x) (1 + c_3 \Delta L(x)) \| y - y' \|, \]

where \( c_4 \) is a positive constant. It then follows that

(6.18)  \[ \| r(x + \Delta, y) - r(x + \Delta, y') \| \]

\[ \leq \Delta \| B \| \| y - y' \| + L(x) \| v(x,y) - v(x',y') \| \]

\[ + 2c_4 \Delta L(x) (1 + c_3 \Delta L(x)) \| y - y' \| \]

\[ \leq [\Delta \| B \| + L(x) [1 + (c_3 + 2c_3c_4) \Delta L(x) + 2c_4 \Delta)] \| y - y' \|. \]

Consequently, (6.6) follows if we define \( L(x + \Delta) \) by the equation

(6.19)  \[ L(x + \Delta) = c_5 \Delta + L(x) (1 + 2c_5 \Delta + c_5 \Delta L(x)), \]

with \( c_5 = \max(\| B \|, c_3 + 2c_3c_4, c_4) \).

From a lemma proved in [6]

(6.20)  \[ L(x) \leq \left[ \frac{1}{1 + L(0) - c_5 x} \right]^{-1} - 1 \]

if
\[ c_5 x \leq 1/(1 + L(0)). \]

In view of (3.4), the induction can be started by taking \( L(0) = L_0 \) and can be continued in the region (6.1) as long as the condition \( \Delta \| B \| L(x) < 1/2 \) is satisfied. By restricting \( x \) to a small enough interval, we obtain from (6.3) the result that \( r(x,y) \) satisfies a Lipschitz condition

\[ \| r(x,y) - r(x,y') \| \leq K \| y - y' \| \]

where \( K \) is independent of \( x \) and \( \Delta \).
REFERENCES


