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A SEMI-DISCRETIZATION ALGORITHM FOR TWO-DIMENSIONAL PARTIAL DIFFERENTIAL EQUATIONS

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A semi-discretization algorithm for two-dimensional partial differential equations

by

J. Kok, P.J. van der Houwen & P.H.M. Wolkenfelt

ABSTRACT

This paper describes the semi-discretization method of a general class of non-linear two-dimensional time-dependent P.D.E.'s on a grid with non-uniform meshes. Secondly, it presents the documentation of the semi-discretization algorithm. Finally, the relation with other semi-discretization methods to be used together with different time-integrators for solving initial-boundary value problems is indicated.

KEY WORDS & PHRASES: *Partial differential equations, Semi-discretization, method of lines.*

CONTENTS

1. INTRODUCTION

A more or less accepted approach of developing software for solving the initial boundary value problem for a time dependent partial differential equation is based on the method of lines or semi-discretization method. Suppose that we are given the initial boundary value problem

$$\frac{\partial U}{\partial t} = G\left(t,x,y,U,\frac{\partial U}{\partial x},\frac{\partial U}{\partial y},\frac{\partial^2 U}{\partial x^2},\frac{\partial^2 U}{\partial x \partial y},\frac{\partial^2 U}{\partial y^2}\right), \qquad t \geq t_0,\ (x,y) \in \Omega$$

$$(1.1) \qquad U(t_0,x,y) = U_0(x,y),\ (x,y) \in \Omega \ ,$$

$$B\left(t,x,y,U,\frac{\partial U}{\partial x},\frac{\partial U}{\partial y}\right) = 0, \qquad t \geq t_0,\ (x,y) \in \partial\Omega$$

where G, U_0 and B are given functions and Ω is a two-dimensional region bounded by one or more closed curves representing the boundary $\partial\Omega$ (see figure 1.1).

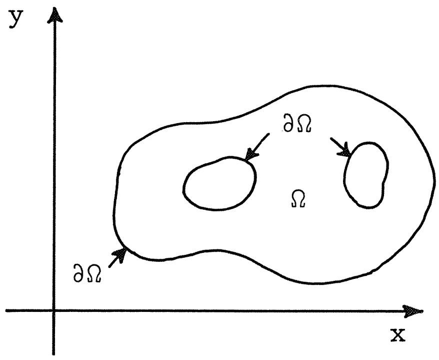

Fig. 1.1 A triply-connected region

The semi-discretization method based on finite differences replaces the derivatives of the unknown function U with respect to the space variables x and y by difference quotients defined on certain sets of grid points R and ∂R belonging to the region Ω and its boundary $\partial\Omega$, respectively. Let U be a grid function defined on $R \cup \partial R$, then semi-discretization of problem (1.1) yields at each (*internal*) grid point of R an ordinary differential equation of the form

$$(1.2) \qquad \frac{d}{dt}\, u(t) = \tilde{G}(t,u), \qquad t \geq t_0$$

with initial conditions

$$(1.3) \qquad u(t_0) = \{U_0(x,y)\}_{(x,y) \in R'}$$

and at each (*boundary*) grid point of ∂R a condition of the form

$$(1.4) \qquad \tilde{B}(t,u) = 0, \qquad t \geq t_0.$$

In this paper we present an algorithm which transforms problem (1.1) into problem (1.2)-(1.4). The transformation is based on divided differences using non-uniform meshes and yields a second order approximation to the original problem (1.1). In order to use the algorithm one should prescribe the functions G, B and U_0, and either the grid points or the grid lines of which the grid points are the points of intersection.

In the last section, it is described in which way we can use the various semi-discretization methods together with time-integrators for the solution of (1.2) - (1.4).

This paper has been written as a contribution to a project of the Numerical Mathematics department of the MC to develop numerical algorithms for the solution of initial boundary value problems.

2. DISCRETIZATIONS ON A CURVILINEAR NET

In the numerical solution of partial differential equations by finite difference methods it is often desirable to approximate the derivatives by difference quotients on a non-uniform grid. The usual derivation of difference quotients by Taylor expansions, however, is rather cumbersome as soon as the grid meshes differ from rectangles (cf. [3]). Therefore, we have chosen an alternative approach. Confining our considerations to discretizations of derivatives in two variables x and y, we introduce two new variables X and Y which are functions of x and y, and which define by the equations

(2.1) $\quad X(x,y) = k\Delta,\ Y(x,y) = r\Delta, \quad k$ and r integers

a curvilinear net in the (x,y)-plane. In the (X,Y)-plane this non-uniform grid is transformed into a uniform grid with square meshes of width Δ (see figures 2.1 and 2.2).

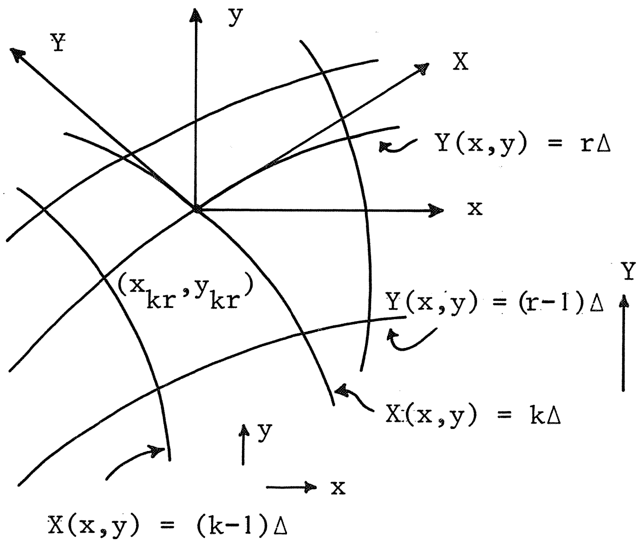

Fig. 2.1 (x,y)-plane

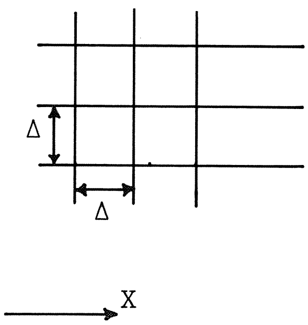

Fig. 2.2 (X,Y)-plane

The coordinates of the grid points in the (x,y)-plane will be denoted by x_{kr} and y_{kr}. Thus,

(2.1) $\quad X(x_{kr},y_{kr}) = k\Delta,\ Y(x_{kr},y_{kr}) = r\Delta.$

Next we express the differential operators with respect to x and y in terms of differential operators with respect to X and Y:

(2.2)
$$\frac{\partial}{\partial x} = \frac{\partial X}{\partial x}\frac{\partial}{\partial X} + \frac{\partial Y}{\partial x}\frac{\partial}{\partial Y},$$
$$\frac{\partial}{\partial y} = \frac{\partial X}{\partial y}\frac{\partial}{\partial X} + \frac{\partial Y}{\partial y}\frac{\partial}{\partial Y},$$
$$\frac{\partial^2}{\partial x^2} = \frac{\partial^2 X}{\partial x^2}\frac{\partial}{\partial X} + \frac{\partial^2 Y}{\partial x^2}\frac{\partial}{\partial Y} + \left(\frac{\partial X}{\partial x}\right)^2\frac{\partial^2}{\partial X^2} + \left(\frac{\partial Y}{\partial x}\right)^2\frac{\partial^2}{\partial Y^2} + 2\,\frac{\partial X}{\partial x}\cdot\frac{\partial Y}{\partial x}\frac{\partial^2}{\partial X\partial Y},$$

$$\frac{\partial^2}{\partial x \partial y} = \frac{\partial^2 X}{\partial x \partial y}\frac{\partial}{\partial X} + \frac{\partial^2 Y}{\partial x \partial y}\frac{\partial}{\partial Y} + \frac{\partial X}{\partial x} \cdot \frac{\partial X}{\partial y}\frac{\partial^2}{\partial X^2} +$$

$$(2.2) \qquad + \frac{\partial Y}{\partial x}\frac{\partial Y}{\partial y}\frac{\partial^2}{\partial Y^2} + \left[\frac{\partial X}{\partial x}\frac{\partial Y}{\partial y} + \frac{\partial Y}{\partial x}\frac{\partial X}{\partial y}\right]\frac{\partial^2}{\partial X \partial Y},$$

$$\frac{\partial^2}{\partial y^2} = \frac{\partial^2 X}{\partial y^2}\frac{\partial}{\partial X} + \frac{\partial^2 Y}{\partial y^2}\frac{\partial}{\partial Y} + \left(\frac{\partial X}{\partial y}\right)^2\frac{\partial^2}{\partial X^2} + \left(\frac{\partial Y}{\partial y}\right)^2\frac{\partial^2}{\partial Y^2} + 2\,\frac{\partial X}{\partial y} \cdot \frac{\partial Y}{\partial y}\frac{\partial^2}{\partial X \partial Y}.$$

Since the differential operators $\partial/\partial X$ and $\partial/\partial Y$ are easily discretized on the square grid shown in figure 2.2, we only have to derive expressions for the derivatives $\partial X/\partial x$, $\partial X/\partial y$, $\partial Y/\partial x$, ... at the grid points (x_{kr}, y_{kr}). In [4] a first order approximation to these quantities is derived. Here, we try to find higher order approximations. We will distinguish two cases: firstly, the case where the grid lines (2.1) are explicitly given and secondly, the case where only the points of intersection of the grid lines are available. The latter case was also considered in [2].

2.1 Formulas using grid lines

In this section it will be assumed that the grid lines defined by (2.1) are explicitly given, that is, we have at our disposal the equations

$$(2.3) \qquad y = f_r(x), \qquad x = g_k(y)$$

presenting the "horizontal" and "vertical" grid lines, respectively.

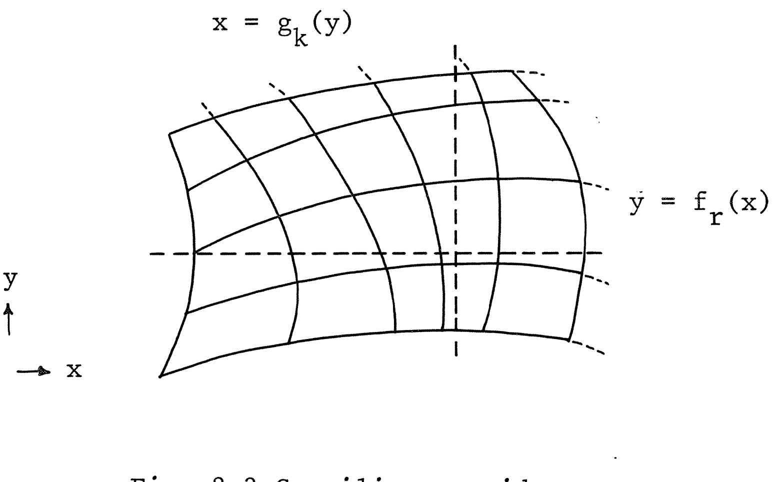

Fig. 2.3 Curvilinear grid

Our problem now is the construction of functions $X(x,y)$ and $Y(x,y)$ with continuous second derivatives and such that

$$X(g_k(y),y) = k\,\Delta\ ,$$
(2.4)
$$Y(x,f_r(x)) = r\,\Delta\ .$$

When we succeed in finding such functions, the operators $\partial/\partial x$, $\partial/\partial y$, ... can be discretized within the accuracy of the discretization of the operators $\partial/\partial X$, $\partial/\partial Y$, ... on the square grid $(k\Delta, r\Delta)$ in the (X,Y)-plane. Consider (2.4) for arbitrary, but fixed values y and x, respectively.

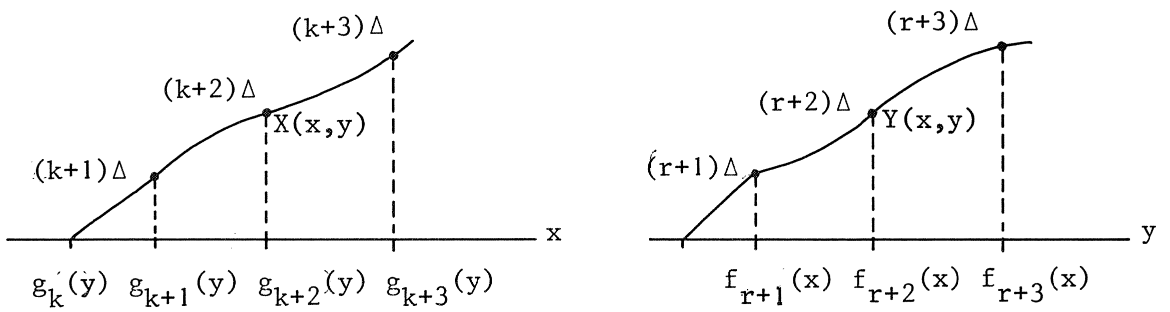

Fig. 2.4. Behaviour of the functions $X(x,y)$ and $Y(x,y)$ when (2.4) is fulfilled.

Then we see that the functions $X(x,y)$ and $Y(x,y)$ are required to have the behaviour as shown in figure 2.4. Moreover, these functions should be twice differentiable at all $x \in [g_{k_{min}}(y), g_{k_{max}}(y)]$ and all $y \in [f_{r_{min}}(x), f_{r_{max}}(x)]$, respectively.

Rather than trying to construct *global* representations of the transformation functions X an Y, we will construct *local* representations in the neighbourhood of the grid lines $x = g_k(y)$ and $y = f_r(x)$. We may then imagine that these representations are sufficiently smoothly continuated and matched together in the "in between" regions. It is tempting to define $X(x,y)$ by a Lagrange polynomial in x:

$$X(x,y) = \sum_{j=k-m_1}^{k+m_2} j\Delta \frac{\prod\limits_{\substack{\ell=k-m_1 \\ \ell\neq j}}^{k+m_2} [x-g_\ell(y)]}{\prod\limits_{\substack{\ell=k-m_1 \\ \ell\neq j}}^{k+m_2} [g_j(y)-g_\ell(y)]}, \tag{2.5}$$

in the neighbourhood of $x = g_k(y)$. However, the partial derivatives of this function, in particular those with respect to y, are difficult to evaluate. A considerably easier evaluation is obtained by writing $X = X(x,y)$ and $Y = Y(x,y)$ implicitly as

$$x = \Psi(X,y), \quad y = \Phi(x,Y), \tag{2.6}$$

and by observing that condition (2.4) transforms into

$$\begin{aligned} g_k(y) &= \Psi(k\Delta,y) \\ f_r(x) &= \Phi(x,r\Delta) \end{aligned} \quad . \tag{2.4'}$$

From these relations it is seen that along the grid lines $x = g_k(y)$ the derivatives of the function Ψ with respect to X can be approximated in an extremely simple manner and similarly the derivatives of Φ with respect to Y along the grid lines $y = f_r(x)$. For instance, along the lines $X(x,y) = k\Delta$, we may write

$$\begin{aligned} \frac{\partial\Psi}{\partial X}(k\Delta,y) &= \frac{g_{k+1}(y) - g_{k-1}(y)}{2\Delta} + O(\Delta^2) \\ \frac{\partial^2\Psi}{\partial X^2}(k\Delta,y) &= \frac{g_{k+1}(y) - 2g_k(y) + g_{k-1}(y)}{\Delta^2} + O(\Delta^2) \end{aligned} \quad \text{as } \Delta \to 0, \tag{2.7}$$

and similar expressions for $\partial\Phi/\partial Y$, $\partial^2\Phi/\partial Y^2$ along the lines $Y(x,y) = r\Delta$.

Having found approximations to the derivatives of Ψ and Φ with respect to X and Y, respectively, we only have to derive relations between these derivatives and the derivatives $\partial X/\partial x$, $\partial^2 X/\partial x^2$, ... occurring in the formulas (2.2). Such relations can be obtained by differentiating equations (2.6) with respect to x and y:

(2.8)
$$1 = \frac{\partial\Psi}{\partial X}\frac{\partial X}{\partial x}\,,\quad 0 = \frac{\partial^2\Psi}{\partial X^2}\left[\frac{\partial X}{\partial x}\right]^2 + \frac{\partial\Psi}{\partial X}\frac{\partial^2 X}{\partial x^2}\,,\quad 0 = \left[\frac{\partial^2\Psi}{\partial X^2}\frac{\partial X}{\partial y} + \frac{\partial^2\Psi}{\partial X\partial y}\right]\frac{\partial X}{\partial x} + \frac{\partial^2 X}{\partial x\partial y}\frac{\partial\Psi}{\partial X}$$
$$1 = \frac{\partial\Phi}{\partial Y}\frac{\partial Y}{\partial y}\,,\quad 0 = \frac{\partial^2\Phi}{\partial Y^2}\left[\frac{\partial Y}{\partial y}\right]^2 + \frac{\partial\Phi}{\partial Y}\frac{\partial^2 Y}{\partial y^2}\,,\quad 0 = \left[\frac{\partial^2\Phi}{\partial Y^2}\frac{\partial Y}{\partial x} + \frac{\partial^2\Phi}{\partial Y\partial x}\right]\frac{\partial Y}{\partial y} + \frac{\partial^2 Y}{\partial x\partial y}\frac{\partial\Phi}{\partial Y}.$$

From (2.7) and (2.8) approximations to the derivatives $\partial X/\partial x$, $\partial^2 X/\partial x^2$, $\partial Y/\partial y$ and $\partial Y^2/\partial y^2$ at the grid points can be derived. In order to find the remaining derivatives we need some additional relations between the derivatives of X and Y. These are provided by differentiating equations (2.4). Along the grid lines we then find

(2.9)
$$\frac{\partial X}{\partial y} = -\,g'_k(y)\,\frac{\partial X}{\partial x}\,,$$
$$\frac{\partial Y}{\partial x} = -\,f'_r(x)\,\frac{\partial Y}{\partial y}\,,$$
$$\frac{\partial^2 X}{\partial y^2} = -\left[g'_k(y)\right]^2\frac{\partial^2 X}{\partial x^2} - 2\,g'_k(y)\,\frac{\partial^2 X}{\partial x\partial y} - g''_k(y)\,\frac{\partial X}{\partial x}\,,$$
$$\frac{\partial^2 Y}{\partial x^2} = -\left[f'_r(x)\right]^2\frac{\partial^2 Y}{\partial y^2} - 2\,f'_r(x)\,\frac{\partial^2 Y}{\partial x\partial y} - f''_r(x)\,\frac{\partial Y}{\partial y}\,.$$

From (2.7) - (2.9) approximations at the grid points can be derived to all derivatives occurring in formula (2.2). In the expressions given below all functions are assumed to be evaluated at the grid point (x_{kr}, y_{kr}) where

(2.10)
$$x_{kr} = g_k(y_{kr}),\qquad y_{kr} = f_r(x_{kr}).$$

Then we may write

(2.11)
$$\frac{\partial X}{\partial x} = \frac{2\Delta}{g_{k+1}-g_{k-1}} + O(\Delta^2),$$
$$\frac{\partial X}{\partial y} = -\,g'_k\,\frac{\partial X}{\partial x}\,,$$

$$
\begin{aligned}
\frac{\partial^2 X}{\partial x^2} &= -\,8\,\frac{g_{k+1} - 2g_k + g_{k-1}}{(g_{k+1}-g_{k-1})^3}\,\Delta + O(\Delta^2)\,,\\
\frac{\partial^2 X}{\partial x \partial y} &= \frac{\partial^2 X}{\partial x^2}\,\frac{\partial X}{\partial y}\left[\frac{\partial X}{\partial x}\right]^{-1} - \left[\frac{\partial X}{\partial x}\right]^{2}\,\frac{g'_{k+1} - g'_{k-1}}{2\Delta} + O(\Delta^2),\\
\frac{\partial^2 X}{\partial y^2} &= -\,\{[g'_k]^2\,\frac{\partial^2 X}{\partial x^2} + 2g'_k\,\frac{\partial^2 X}{\partial x \partial y} + g''_k\,\frac{\partial X}{\partial x}\,\},
\end{aligned}
\tag{2.11}
$$

and similar expressions for the derivatives of Y.

The expressions given in (2.11) only apply to grid points (x_{kr}, y_{kr}) for which the functions g_{k-1}, g_{k+1}, f_{r-1} and f_{r+1} are available. Thus, (2.11) applies to boundary grid points provided that the neighbouring *external* grid line is also prescribed (see figure 2.5).

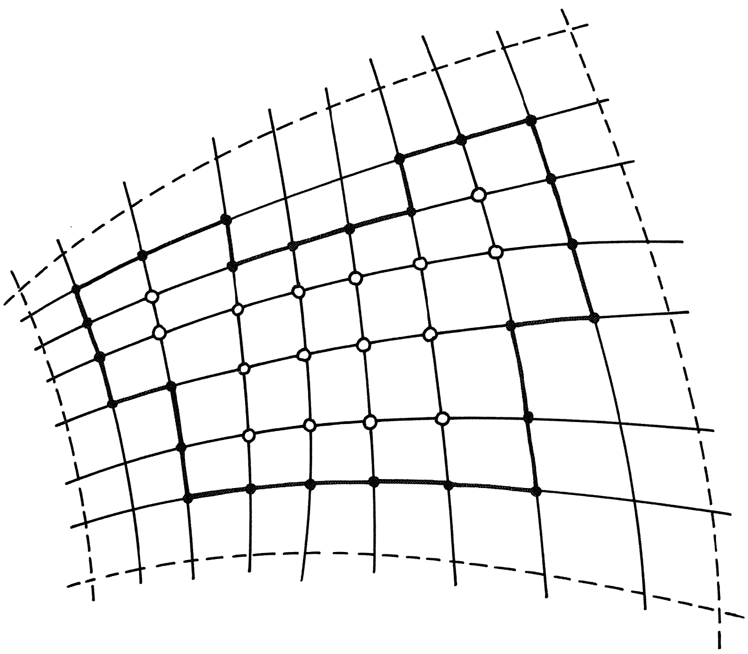

Fig. 2.5. External grid lines (- - -)

An alternative would be the definition of asymmetric difference approximations to the derivatives $\partial\Psi/\partial X$, $\partial^2\Psi/\partial X^2$,... (cf. (2.7)) at the boundary points. For instance, along a "left" boundary grid line $X(x,y) = k\Delta$, we may define

$$\frac{\partial \Psi}{\partial X}(k\Delta,y) = \frac{-3g_k + 4g_{k+1} - g_{k+2}}{2\Delta} + O(\Delta^2)$$

$$(2.7') \qquad \frac{\partial^2 \Psi}{\partial X^2}(k\Delta,y) = \frac{2g_k - 5g_{k+1} + 4g_{k+2} - g_{k+3}}{\Delta^2} + O(\Delta^2) \qquad \text{as } \Delta \to 0.$$

The expressions in (2.11) which are changed by using (2.7') instead of (2.7) are given by

$$\frac{\partial X}{\partial x} = \frac{2\Delta}{-3g_k + 4g_{k+1} - g_{k+2}} + O(\Delta^2),$$

$$(2.11') \qquad \frac{\partial^2 X}{\partial x^2} = -8\,\frac{2g_k - 5g_{k+1} + 4g_{k+2} - g_{k+3}}{(-3g_k+4g_{k+1}-g_{k+2})^3}\,\Delta + O(\Delta^2),$$

$$\frac{\partial^2 X}{\partial x \partial y} = \frac{\partial^2 X}{\partial x^2}\frac{\partial X}{\partial y}\left[\frac{\partial X}{\partial y}\right]^{-1} - \left[\frac{\partial X}{\partial x}\right]^2 \frac{-3g'_k + 4g'_{k+1} - g'_{k+2}}{2\Delta} + O(\Delta^2).$$

2.2 Formulas using only grid points

In the preceding section the availability of a twice differentiable representation of the grid lines was assumed. In many cases, however, we only have the coordinates of the grid points at our disposal. Expressions (2.11) may still be used when the quantities g_{k+1}, g_{k-1}, g'_{k+1}, g'_k, g'_{k-1} and g''_k are replaced by numerical approximations in terms of the grid point coordinates (see figure 2.6).

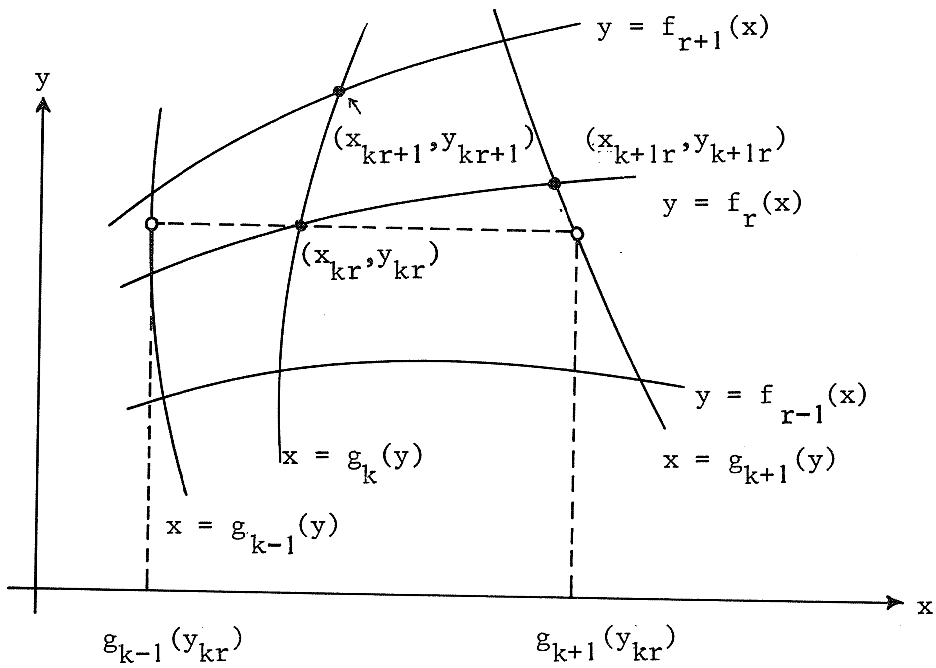

fig. 2.6 Situation at the grid point (x_{kr}, y_{kr})

Suppose that we are given the slope $g'_\ell(y_{\ell r})$ and curvature $g''_\ell(y_{\ell r})$ of the grid line $x = g_\ell(y)$ in all grid points $(x_{\ell r}, y_{\ell r})$. Then we may use the approximations

$$
(2.12)\qquad
\begin{aligned}
g'_\ell(y_{kr}) &= g'_\ell(y_{\ell r}) + (y_{kr}-y_{\ell r})\, g''_\ell(y_{\ell r}) + O(\Delta^2),\\
g_\ell(y_{kr}) &= x_{\ell r} + (y_{kr}-y_{\ell r})\, g'_\ell(y_{\ell r}) + \tfrac{1}{2}(y_{kr}-y_{\ell r})^2\, g''(y_{\ell r}) + O(\Delta^3),
\end{aligned}
$$

where $\ell = k-1,\ k,\ k+1$ in case of (2.11) and $\ell = k,\ k+1,\ k+2,\ k+3$ in case of (2.11').

Finally, the values of $g'_k(y_{kr})$ and $g''_k(y_{kr})$ are to be approximated. Using three reference points we obtain

$$
(2.13)\qquad
\begin{aligned}
g''_k(y_{kr}) &= 2\left[\frac{\Delta x_{kr}}{\Delta y_{kr}} - \frac{\Delta x_{kr-1}}{\Delta y_{kr-1}}\right]\left[\Delta y_{kr} + \Delta y_{kr-1}\right]^{-1} + O(\Delta),\\
g'_k(y_{kr}) &= \frac{\Delta x_{kr}}{\Delta y_{kr}} - \tfrac{1}{2}\,\Delta y_{kr}\, g''_k(y_{kr} + O(\Delta^2)
\end{aligned}
$$

where $\Delta x_{kr} = x_{kr+1} - x_{kr}$ and $\Delta y_{kr} = y_{kr+1} - y_{kr}$. In order to get second order approximations to $g''_k(y_{kr})$ one should use at least four reference points. Let us write

$$
(2.14)\qquad g''_k(y_{kr}) \cong \sum_{j=-3}^{+3} a_j\, x_{kr+j},
$$

then this expression is *second order accurate* when the coefficient vector $\vec{a} = (a_j)$ satisfies the equation

$$
(2.15)\qquad
\begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1\\
-\Delta_{r-3} & -\Delta_{r-2} & -\Delta_{r-1} & 0 & \Delta_{r+1} & \Delta_{r+2} & \Delta_{r+3}\\
\Delta^2_{r-3} & \Delta^2_{r-2} & \Delta^2_{r-1} & 0 & \Delta^2_{r+1} & \Delta^2_{r+2} & \Delta^2_{r+3}\\
-\Delta^3_{r-3} & -\Delta^3_{r-2} & -\Delta^3_{r-1} & 0 & \Delta^3_{r+1} & \Delta^3_{r+2} & \Delta^3_{r+3}
\end{pmatrix}
\vec{a} =
\begin{pmatrix} 0\\ 0\\ 2\\ 0 \end{pmatrix},
$$

where $\Delta_{r+j} = |y_{kr+j}-y_{kr}|$. The first derivative $g'_k(y_{kr})$ is then still given by (2.13) with second order accuracy. The approximation (2.14) - (2.15) can be used at

$$\left.\begin{array}{l}\text{lefthand boundary points}\\ \text{righthand boundary points}\\ \text{"almost" lefthand boundary points}\\ \text{"almost" righthand boundary points}\\ \text{remaining internal points}\end{array}\right\}\text{by choosing}\left\{\begin{array}{l}a_{-3}=a_{-2}=a_{-1}=0\\ a_3=a_2=a_1=0\\ a_{-3}=a_{-2}=a_3=0\\ a_3=a_2=a_{-3}=0\\ a_{-3}=a_3=0\end{array}\right.$$

2.3 Approximation of the original differential operators

Having derived numerical approximations to the derivatives of the transformation functions X and Y, we are able to define the difference approximations to the *original* differential operators. Let us approximate the differential operators in the coordinates X and Y by *central differences* and write

$$\frac{\partial X}{\partial x}=X_1\Delta,\ \frac{\partial X}{\partial y}=X_2\Delta,\ \frac{\partial^2 X}{\partial x^2}=X_{11}\Delta,\ \frac{\partial^2 X}{\partial y^2}=X_{22}\Delta,\ \frac{\partial^2 X}{\partial x\partial y}=X_{12}\Delta,$$

(2.16)

$$\frac{\partial Y}{\partial x}=Y_1\Delta,\ \frac{\partial Y}{\partial y}=Y_2\Delta,\ \frac{\partial^2 Y}{\partial x^2}=Y_{11}\Delta,\ \frac{\partial^2 Y}{\partial y^2}=Y_{22}\Delta,\ \frac{\partial^2 Y}{\partial x\partial y}=Y_{12}\Delta.$$

From (2.2) it then can be derived that second order accurate approximations $[\partial/\partial x]$, $[\partial/\partial y]$,... to $\partial/\partial x$, $\partial/\partial y$,... are given by the following "molecule" representations:

$$\left[\frac{\partial}{\partial x}\right]=\frac{1}{2}\begin{bmatrix}0 & Y_1 & 0\\ -X_1 & 0 & X_1\\ 0 & -Y_1 & 0\end{bmatrix},\quad \left[\frac{\partial}{\partial y}\right]=\frac{1}{2}\begin{bmatrix}0 & Y_2 & 0\\ -X_2 & 0 & X_2\\ 0 & -Y_2 & 0\end{bmatrix},$$

$$\left[\frac{\partial^2}{\partial x^2}\right]=\frac{1}{2}\begin{bmatrix}-X_1Y_1 & 2Y_1^2+Y_{11} & X_1Y_1\\ 2X_1^2-X_{11} & -4(X_1^2+Y_1^2) & 2X_1^2+X_{11}\\ X_1Y_1 & 2Y_1^2-Y_{11} & -X_1Y_1\end{bmatrix},$$

$$\left[\frac{\partial^2}{\partial x \partial y}\right] = \frac{1}{2} \begin{bmatrix} -\frac{1}{2}(X_1Y_2+X_2Y_1) & 2Y_1Y_2 + Y_{12} & \frac{1}{2}(X_1Y_2+X_2Y_1) \\ 2X_1X_2 - X_{12} & -4(X_1X_2+Y_1Y_2) & 2X_1X_2 + X_{12} \\ \frac{1}{2}(X_1Y_2+X_2Y_1) & 2Y_1Y_2 - Y_{12} & -\frac{1}{2}(X_1Y_2+X_2Y_1) \end{bmatrix},$$

$$\left[\frac{\partial^2}{\partial y^2}\right] = \frac{1}{2} \begin{bmatrix} -X_2Y_2 & 2Y_2^2 + Y_{22} & X_2Y_2 \\ 2X_2^2 - X_{22} & -4(X_2^2+Y_2^2) & 2X_2^2 + X_{22} \\ X_2Y_2 & 2Y_2^2 - Y_{22} & -X_2Y_2 \end{bmatrix}.$$

CONCLUDING REMARKS

The project for developing numerical algorithms for the solution of initial boundary value problems has resulted in a modular construction of a class of algorithms.

One module is the calculation of approximations of the space derivatives for the right hand side evaluations, one other module is one of the available integrators for the time-integration of the resulting transformed problem (1.2) - (1.4), and finally an interface provides for the representation of the grid, the solution of the boundary condition and the control of all subprocesses involved. In this setup several methods for approximating the space derivatives can easily be exchanged and the same holds for the various time-integrators we want to apply.

In an earlier version of this construct the formulas given in Section 2.3 were used. Together with several time-integrators for semi-discretized parabolic equations, this version was run with several test problems for various grids and boundaries. Here the main advantage of the construct became clear, i.e. the possibility to process problems with all kinds of rectangular as well as curvilinear grids and with unlimitedly kinked boundaries.

Following the conclusions of a comparison by DEKKER (see [1]) it was decided that a later version of the algorithm would be realized with Dekker's method for minimizing the truncation errors of the derivative approximations, at the same time allowing a wider class of boundary conditions. The main reason for this exchange was the expected better approximation of the space derivatives on curvilinear grids, although Dekker's method proved to be more expensive in both computation time and memory. Results of tests with Dekker's semi-discretization method will be given in the near future.

The realization of the algorithm, containing now Dekker's method and an interface for delivering right hand side evaluations of the initial value problem originated by semi-discretization, is described in [5]. The semi-discretization method is exchangeable, while the time-integrator is a parameter of the algorithm. In this shape the algorithm will be used for the investigations at the Mathematical Centre of suitable time-integrators for problems originated from initial boundary value problems.

It is clear that Dekker's method, using nine grid points only for approximating derivatives, uses less information than the here described discretization method that has the possibility to derive the transformation function for transforming the real space (containing the grid and the grid lines) to the discretization space where the grid is uniform with square meshes. It can use the complete grid lines and it is not restricted to sub-grids of three horizontal and vertical lines for computing the approximations locally. It is therefore expected that the method presented here will be important in the proceeding investigations of methods for solving initial boundary value problems.

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