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Kernel Optimum Nearly-analytical Discretization (KOND) Method Applied to Parabolic Equations ≪ KOND-P Scheme ≫

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Abstract

A KOND-P scheme, which is the application of the Kernel Optimum Nearly-analytical Discretization (KOND) method for the construction of numerical schemes to the parabolic type partial differential equation, is presented. Typical numerical results are shown to clarify that the KOND-P scheme yields quite less numerical error than the conventional explicit scheme by 2 - 3 orders measured by the root mean square deviation from analytical solutions.

Keywords : thought analysis, numerical scheme, KOND method, KOND-P scheme, parabolic type equation,KOND-H scheme, high accuracy, Taylor expansion, kernel optimum discretization.

§ 1. Inroduction

Various numerical algorithms for solving the three types of partial differential problems of hyperbolic, elliptic and parabolic equations have been developed.[1-11] While they yield fairly good results for many problems, more effort will be required to attain higher accuracy and stability when we investigate further the finer structure of the problem being studied. One of the authors has reported a thought analysis on numerical schemes and developed a new method called "Kernel Optimum Nearly-analytical Discretization (KOND) method" for the construction of numerical schemes.[12] In the thought analysis, we investigate logical structures, ideas or thoughts used in the objects being studied, and try to find some key elements for improvement and/or some other new thoughts which involve generality.[12-14] In the previous report,[12] the 2nd order KOND-H scheme, which is one of the applications of the KOND method to the numerical scheme for solving the hyperbolic type equation to the 2nd derivatives, has been shown in detail. It has been demonstrated by the numerical results of the 2nd order KOND-H scheme that the KOND-H scheme yields fairly less diffusive error compared with other conventional schemes and has fairly high stability.[12] It has been also demonstrated by the numerical results that there appears higher diffusive error and/or noise in the calculation of the higher derivatives of the solutions. This structural property of the error would be common in all numerical schemes. A brief description of another application of the KOND method to the parabolic type equation (called "the KOND-P scheme") has been also shown as a demonstration for the wide applicability of the new method in the previous report.[12] In this paper, we present in detail the KOND-P scheme with a treatment of the boundary values of higher derivatives and show numerical results by the KOND-P scheme comparing with those by the conventional explicit scheme. Numerical examples by the KOND-P scheme show quite less numerical error than those by the conventional one by 2 - 3 orders measured by the root mean square deviation from analytical solutions.

In §2, the KOND method deduced from the thought analysis on numerical schemes is shown briefly. The 1st order KOND-P scheme, which is the application of the KOND method to the numerical scheme for solving the parabolic type equation to the 1st derivatives, is presented in detail in §3 together with the treatment of the boundary values of higher derivatives. Numerical results by the 1st order KOND-P scheme are given in §4 together with discussion comparing with those by the conventional explicit scheme.

§ 2. KOND Method deduced from Thought Analysis on Numerical Schemes

We present here briefly the thought analysis on numerical schemes to lead to the KOND method.[12] In order to understand the structure of the ideas or thoughts used for numerical schemes for simulation, we try to analyse the basic process for solving a partial differential problem,

$$Lf(\mathbf{x}) = g(\mathbf{x}), \text{ for } \mathbf{x} = (x_1, \cdots, x_d) \text{ in a domain } \Omega \subset R^d, \tag{1}$$

where L is a linear or nonlinear differential operator, $f(\mathbf{x})$ is an unknown function, and $g(\mathbf{x})$ is a given function. When it is hard to solve analytically Eq.(1), we use usually two approximate methods, i.e. one is the approximate analytic method such as the perturbation method and the other is the discretization of Eq.(1) to solve the finite-difference equations. When we compare the ideas or thoughts themselves involved in the two methods, we may find the following elements of thoughts (we call the idea or thought itself involved in some method, simply like as " thought [A] ").

In the approximate analytic method:

[A] to find global approximate continuous solutions.

[B] to find local approximate continuous solutions.

In the discretization method:

[C] to find finite-difference equations approximately equal to source equations.

[D] to find discrete approximate solutions on grids.

Since the finite-difference equation for Eq.(1) itself has finite error compared with the source equation, Eq.(1), we had better solve Eq.(1) directly as possible, avoiding to use the finite-difference equation.

We now assume here that the analytic true solution $f(\mathbf{x})$ of Eq.(1) is obtained. The whole informations that give the whole property or character of Eq.(1) and its solution are included in the following set of the analytic solution and its derivatives,

$$\{\ f(\mathbf{x}),\ \partial_i f(\mathbf{x}),\ \partial_{ij} f(\mathbf{x}),\ \cdots\ \}, \tag{2}$$

where $\partial_i f(\mathbf{x})$, $\partial_{ij} f(\mathbf{x}), \cdots$ stand respectively for $\partial f(\mathbf{x})/\partial x_i$, $\partial^2 f(\mathbf{x})/\partial x_i \partial x_j$, and so on. The each element of the set of Eq.(2) obeys respectively the following set of differential equations,

$$\{\ \text{Eq.}(1),\ \text{Eq.}(4),\ \text{Eq.}(5),\ \cdots\ \}, \tag{3}$$

where Eqs.(4), (5), $\cdots$, are the followings;

$$\partial_i[\ Lf(\mathbf{x}) = g(\mathbf{x})\ ], \quad \text{for } \mathbf{x} = (x_1, \cdots, x_d), \tag{4}$$

$$\partial_{ij}[\ Lf(\mathbf{x}) = g(\mathbf{x})\ ], \quad \text{for } \mathbf{x} = (x_1, \cdots, x_d), \tag{5}$$

....

We call Eq.(1) "the source equation", Eq.(4) "the first branch equations", Eq.(5) "the second branch equations" , and so on.

Mapping the set of analytic solutions, Eq.(2), onto the grid points $\mathbf{x}_n^h$ in a given uniform or nonuniform grid G^h with mesh size $\mathbf{h}_d$, we may obtain the following set of { discrete values of solutions at grid points, interpolation curves around grid points, connection relations at neighboring grid points } which is equivalent to the set of Eq.(2):

⟨ *set of discrete values of solutions at grid points* ⟩

$$\{ \ f_n, \ \partial_i f_n, \ \partial_{ij} f_n, \ \cdots \}, \tag{6}$$

where the subscript n denotes here a d dimensional integer.

⟨ *set of interpolation curves around grid points* ⟩

$$\{ \ F_n(\mathbf{s}), \ \partial_i F_n(\mathbf{s}), \ \partial_{ij} F_n(\mathbf{s}), \ \cdots \}, \tag{7}$$

where s is defined as $\mathbf{s} \equiv \mathbf{x} - \mathbf{x}_n^h$.

⟨ *set of connection relations at neighboring grid points* ⟩

$$F_n(-\mathbf{h}_d) = f_{n-1}. \qquad F_n(\mathbf{h}_d) = f_{n+1}. \tag{8}$$

$$\partial_i F_n(-\mathbf{h}_d) = \partial_i f_{n-1}. \qquad \partial_i F_n(\mathbf{h}_d) = \partial_i f_{n+1}. \tag{9}$$

$$\partial_{ij} F_n(-\mathbf{h}_d) = \partial_{ij} f_{n-1}. \qquad \partial_{ij} F_n(\mathbf{h}_d) = \partial_{ij} f_{n+1}. \tag{10}$$

....

Each element of the set, Eq.(7), should be the piecewise segment of the corresponding analytical solutions of Eq.(2). The set of { the discrete solutions Eq.(6), the segmental interpolation curves Eq.(7), the connection relations of Eqs.(8), (9), (10), $\cdots$ } is exactly equivalent to the set of the true solutions, Eq.(2). Using the Taylor expansion, the elements of the set of the interpolation curves, Eq.(7), can be written as follows;

$$F_n(\mathrm{s}) = f_n + \sum_i \partial_i f_n s_i + \sum_{i,j} \partial_{ij} f_n s_i s_j/2 + \cdots, \tag{11}$$

$$\partial_i F_n(\mathrm{s}) = \partial_i f_n + \sum_j \partial_{ij} f_n s_j + \sum_{j,k} \partial_{ijk} f_n s_j s_k/2 + \cdots, \tag{12}$$

$$\partial_{ij} F_n(\mathrm{s}) = \partial_{ij} f_n + \sum_k \partial_{ijk} f_n s_k + \sum_{k,l} \partial_{ijkl} f_n s_k s_l/2 + \cdots, \tag{13}$$

....

We see from Eq.(6) and Eqs.(11), (12), (13), $\cdots$ that the discrete values of solution, Eq.(6), are themselves the coefficients of the interpolation curves by the Taylor expansion and therefore induce good approximate and locally continuous solutions around the grid points. In other words, the set of the discrete values of Eq.(6) itself becomes one of the best discretization for the whole informations of the continuous true solutions, Eq.(2). This corresponds analogically to the representation of a given function by the discrete spectra with use of the Fourier expansion. Since we cannot use the infinite elements of the set of Eq.(6), we use two or three elements from the beginning in Eq.(6), for example, f_n, $\partial_i f_n$, $\partial_{ij} f_n$. We then lose finer informations included in the rest infinite terms beyond the terms of $\partial_{ij} f_n$, in this example, in the Taylor expansions. The rest infinite terms are considered to carry the semiglobal informations for the uncovered regions between the neighboring grid points that make the interpolation curves satisfy the connection relations of Eqs.(8) - (10). Using reversely the connection relations and introducing additional Taylor coefficients, i.e. three more additional terms for one dimensional problem in this example, we can recover approximately the lost informations in the rest infinite terms by the additional terms. In other words, the rest infinite terms in the Taylor expansions can be folded up approximately in the finite additional terms by using the connection relations. We then notice that if we have a method which is nearly analytical for obtaining better approximate solutions for the more elements of the set of Eq.(6), we would get the more accurate and denser informations for the set of the true solution, Eq.(2). The accuracy of the informations for the solutions by this method is optimum at the grid points, as is seen from the above argument, and in other words, the discretization by this method is kernel optimum.

The thought analysis mentioned above leads to the following main set of thoughts to be used in the method for the construction of the numerical scheme, which is the combination of the elements of the two sets of thoughts for the approximate analytic method { [A], [B] } and the discretization method { [C], [D] }. We call the method "Kernel Optimum Nearly-analytical Discretization (KOND) method".

Main set of thoughts of the KOND method;

$$\{ [\,\mathrm{I}\,], [\mathrm{II}], [\mathrm{III}], [\mathrm{IV}] \}, \tag{14}$$

where the four elements of thought are as follows,

[I] to use the source equations and their branch equations { Eq.(1), Eq.(4), Eq.(5), $\cdots$ }.

[II] to find high-order approximate analytic solutions by using some methods such as the perturbation method, the Taylor expansion and others.

[III] to find the set of discrete solutions $\{ f_n,\ \partial_i f_n,\ \partial_{ij} f_n,\ \cdots \}$ that are the coefficients of the interpolation curves { Eqs.(11), (12), (13), $\cdots$ } by the Taylor expansions corresponding to the local continuous solutions around the grid points. [The kernel optimum discretization of a function by the coefficients of the Taylor expansion at every grid point.]

[IV] to use the set of the connection relations { Eqs.(8), (9), (10), $\cdots$ } in order to include the semiglobal informations for the uncovered regions between the neighboring gird points and to find the additional higher order Taylor coefficients which represent approximately the rest of the infinite terms of the Taylor expansion. [Folding of rest terms of the Taylor expansion by the connection relations.]

In the following section, we will apply the set of thoughts of the KOND method { [I], [II], [III], [IV] } to the numerical schemes for solving the partial differential problem of parabolic equations.

§ 3. 1st Order KOND Method for Parabolic Equations (1st order KOND – P Scheme)

We apply here the KOND method to the numerical scheme for solving the parabolic type equation. For simplicity, we treat here one dimensional parabolic equation used for diffusion equations, and develop a scheme to obtain the discrete solutions to the 1st derivatives, i.e. f_n and $\partial_x f_n$. Here, the notations such as $\partial_t Y$, $\partial_x Y$, and $\partial_{xx} Y$ denote $\partial Y(t,x)/\partial t$, $\partial Y(t,x)/\partial x$, and $\partial^2 Y(t,x)/\partial x^2$, respectively.

According to the first thought element, [I], of Eq.(14), and from Eq.(4), the source equation and the 1st branch equation for the diffusion equation are written as follows:

$$\partial_t f = P, \tag{15}$$

$$\partial_t(\partial_x f) = \partial_x P, \tag{16}$$

$$P \equiv \partial_x[\, D(t,x)\partial_x f \,], \tag{17}$$

where $D(t,x)$ is a given diffusion coefficient. The m-th branch equation for Eq.(15) is written generally as

$$\partial_t(\partial_{mx} f) = \partial_{mx} P, \tag{18}$$

where $\partial_{mx} f$ is an abbreviation for $\partial^m f/\partial x^m$.

According to the second thought element, [II], of Eq.(14), we solve Eqs.(15) - (17) locally around a point of (t_k, x_n). Using the Taylor expansion around the time of t_k, we write $\partial_{mx} P_n$ as

$$\partial_{mx} P_n \;=\; \partial_{mx} P_n^k \;+\; \partial_{tmx} P_n^k \tau \;+\; ...... \,, \tag{19}$$

where $\tau \equiv t - t_k$, $\partial_{mx} P_n \equiv \partial_{mx} P(t, x_n)$, and $\partial_{mx} P_n^k \equiv \partial_{mx} P(t_k, x_n)$. When $m = 0$ in Eq.(19), then Eq.(19) becomes the Taylor expansion for P itself. Using Eq.(19) and integrating Eqs.(15) and (16) with respect to τ over the time interval of Δt, we obtain approximate solutions for f_n^{k+1} and $\partial_x f_n^{k+1}$ at the point of (t_{k+1}, x_n) as follows,

$$f_n^{k+1} \;=\; f_n^k + P_n^k \Delta t + \partial_t P_n^k (\Delta t)^2/2 + \;......, \tag{20}$$

$$\partial_x f_n^{k+1} \;=\; \partial_x f_n^k + \partial_x P_n^k \Delta t + \partial_{tx} P_n^k (\Delta t)^2/2 + \;......, \tag{21}$$

where $f_n^k \equiv f(t_k, x_n)$ and $\partial_x f_n^k \equiv \partial_x f(t_k, x_n)$.

We now proceed to the third thought element, [III], of Eq.(14). Using the definition of Eq.(17), $P_n^k, \partial_t P_n^k, \partial_x P_n^k$ and $\partial_{tx} P_n^k$ in Eqs.(20) and (21) are given as follows,

$$P_n^k \;=\; \partial_x D_n^k \partial_x f_n^k + D_n^k \partial_{2x} f_n^k, \tag{22}$$

$$\partial_t P_n^k \;=\; \partial_{tx} D_n^k \partial_x f_n^k + \partial_x D_n^k \partial_{tx} f_n^k + \partial_t D_n^k \partial_{2x} f_n^k + D_n^k \partial_{t2x} f_n^k, \tag{23}$$

$$\partial_x P_n^k \;=\; \partial_{2x} D_n^k \partial_x f_n^k + 2\partial_x D_n^k \partial_{2x} f_n^k + D_n^k \partial_{3x} f_n^k, \tag{24}$$

$$\begin{aligned}\partial_{tx} P_n^k \;=\; & \partial_{t2x} D_n^k \partial_x f_n^k + \partial_{2x} D_n^k \partial_{tx} f_n^k + 2\partial_{tx} D_n^k \partial_{2x} f_n^k + 2\partial_x D_n^k \partial_{t2x} f_n^k \\ & + \partial_t D_n^k \partial_{3x} f_n^k + D_n^k \partial_{t3x} f_n^k,\end{aligned} \tag{25}$$

Using Eq.(18), we obtain $\partial_{tx} f_n^k$, $\partial_{t2x} f_n^k$ and $\partial_{t3x} f_n^k$ in Eqs.(23) and (25) in the following forms,

$$\begin{aligned}\partial_{tx} f_n^k &= \partial_x P_n^k \\ &= \partial_{2x} D_n^k \partial_x f_n^k + 2\partial_x D_n^k \partial_{2x} f_n^k + D_n^k \partial_{3x} f_n^k,\end{aligned} \tag{26}$$

$$\begin{aligned}\partial_{t2x} f_n^k &= \partial_{2x} P_n^k \\ &= \partial_{3x} D_n^k \partial_x f_n^k + 3\partial_{2x} D_n^k \partial_{2x} f_n^k + 3\partial_x D_n^k \partial_{3x} f_n^k + D_n^k \partial_{4x} f_n^k,\end{aligned} \tag{27}$$

$$\begin{aligned}\partial_{t3x} f_n^k &= \partial_{3x} P_n^k \\ &= \partial_{4x} D_n^k \partial_x f_n^k + 4\partial_{3x} D_n^k \partial_{2x} f_n^k + 6\partial_{2x} D_n^k \partial_{3x} f_n^k + 4\partial_x D_n^k \partial_{4x} f_n^k + D_n^k \partial_{5x} f_n^k,\end{aligned} \tag{28}$$

Using the values at the time of t_k and/or t_{k-1}, we obtain the derivatives of D, for example, $\partial_t D_n^k = (D_n^k - D_n^{k-1})/\Delta t$, $\partial_x D_n^k = (D_{n+1}^k - D_{n-1}^k)/2h$, and so on, where $h\ (= x_n - x_{n-1}\ )$ is the mesh size. When we use the approximate solutions for f_n^{k+1} and $\partial_x f_n^{k+1}$ to the order of $(\Delta t)^2$ in Eqs.(20) and (21), we can determine the values of f_n^{k+1} and $\partial_x f_n^{k+1}$ with use of Eqs.(22) - (28), the values of D at the time of t_k and/or t_{k-1}, and the values of $\partial_{mx} f_n^k$ $(m = 0, 1, 2, 3, 4, 5)$.

We proceed to the final thought element, [IV], of Eq.(14). Since we have to determine the values of f_n^{k+1} and $\partial_x f_n^{k+1}$ from those of f_n^k and $\partial_x f_n^k$, we need the values of $\partial_{mx} f_n^k$ $(m = 2, 3, 4, 5)$ included in Eqs.(22) - (28). We therefore use the following interpolation curves up to the term of $\partial_{5x} f_n^k$ of the Taylor expansion,

$$\begin{aligned}F_n^k(s) = f_n^k + \partial_x f_n^k s + \partial_{2x} f_n^k s^2/2 + \partial_{3x} f_n^k s^3/6 \\ + \partial_{4x} f_n^k s^4/24 + \partial_{5x} f_n^k s^5/120,\end{aligned} \tag{29}$$

$$\begin{aligned}\partial_x F_n^k(s) = \partial_x f_n^k + \partial_{2x} f_n^k s + \partial_{3x} f_n^k s^2/2 + \partial_{4x} f_n^k s^3/6 \\ + \partial_{5x} f_n^k s^4/24.\end{aligned} \tag{30}$$

We use following four connection relations for f_n^k and $\partial_x f_n^k$ from Eqs.(8) and (9) in order to determine the values of $\partial_{mx} f_n^k$ $(m = 2, 3, 4, 5)$ by f_n^k and $\partial_x f_n^k$,

$$F_n^k(-h) = f_{n-1}^k, \tag{31}$$

$$F_n^k(h) = f_{n+1}^k, \tag{32}$$

$$\partial_x F_n^k(-h) = \partial_x f_{n-1}^k, \tag{33}$$

$$\partial_x F_n^k(h) = \partial_x f_{n+1}^k, \tag{34}$$

Substituting Eqs.(29) and (30) into Eqs.(31) - (34), we obtain the four additional Taylor coefficients, $\partial_{mx} f_n^k$ $(m = 2, 3, 4, 5)$, which are given by f_n^k and $\partial_x f_n^k$, as follows,

$$\partial_{2x} f_n^k = 2(f_{n+1}^k - 2f_n^k + f_{n-1}^k)/h^2 - (\partial_x f_{n+1}^k - \partial_x f_{n-1}^k)/2h, \tag{35}$$

$$\partial_{3x} f_n^k = 15(f_{n+1}^k - f_{n-1}^k)/2h^3 - 3(\partial_x f_{n+1}^k + 8\partial_x f_n^k + \partial_x f_{n-1}^k)/2h^2, \tag{36}$$

$$\partial_{4x} f_n^k = -12(f_{n+1}^k - 2f_n^k + f_{n-1}^k)/h^4 + 6(\partial_x f_{n+1}^k - \partial_x f_{n-1}^k)/h^3, \tag{37}$$

$$\partial_{5x} f_n^k = -90(f_{n+1}^k - f_{n-1}^k)/h^5 + 30(\partial_x f_{n+1}^k + 4\partial_x f_n^k + \partial_x f_{n-1}^k)/h^4, \tag{38}$$

Using the initial values of f_n, i.e. f_n^1, we obtain the initial values of $\partial_x f_n$, i.e. $\partial_x f_n^1$, by $\partial_x f_n^1 = (f_{n+1}^1 - f_{n-1}^1)/2h$.

We now consider how to treat the boundary values of f_n^k and $\partial_x f_n^k$. The boundary conditions for the source equation, Eq.(15), are given usually in one of the following two forms,

$$\text{boundary condition (a)}: \qquad f_n^k = \text{const.} \quad (n = 1, N), \tag{39}$$

$$\text{boundary condition (b)}: \qquad \partial_x f_n^k = \text{const.} \quad (n = 1, N), \tag{40}$$

where ($n = 1$ and $n = N$) denote the boundary grids. We show here how to determine the values of $\partial_x f_n^k$ ($n = 1, N$) for the case of the boundary condition (a) of Eq(39). [If we use the boundary condition (b) of Eq.(40), then we exchange f_1^k with $\partial_x f_1^k$ in the following argument.] According to the thought elements [III] and [IV] of Eq.(14), the interpolation curve around the grid point x_2 and the connection relations are given respectively from Eqs.(29) and (30) and Eqs.(31) - (34) as follows,

$$F_2^k(s) = f_2^k + \partial_x f_2^k s + \partial_{2x} f_2^k s^2/2 + \partial_{3x} f_2^k s^3/6 \\ + \partial_{4x} f_2^k s^4/24 + \partial_{5x} f_2^k s^5/120, \tag{41}$$

$$\partial_x F_2^k(s) = \partial_x f_2^k + \partial_{2x} f_2^k s + \partial_{3x} f_2^k s^2/2 + \partial_{4x} f_2^k s^3/6 \\ + \partial_{5x} f_2^k s^4/24. \tag{42}$$

$$F_2^k(-h) = f_1^k, \tag{43}$$

$$F_2^k(h) = f_3^k, \tag{44}$$

$$\partial_x F_2^k(-h) = \partial_x f_1^k, \tag{45}$$

$$\partial_x F_2^k(h) = \partial_x f_3^k. \tag{46}$$

Since $\partial_x f_1^k$ is unknown this time in addition to $\partial_{mx} f_2^k$ $(m = 2, 3, 4, 5)$, we have to remove the last term of $\partial_{5x} f_2^k$ in Eqs.(41) and (42). Substituting Eqs.(41) and (42) without the term of $\partial_{5x} f_2^k$ into Eqs.(43) - (46), we obtain the three additional Taylor coefficients, $\partial_{mx} f_2^k$ $(m = 2, 3, 4)$, and $\partial_x f_1^k$, as follows,

$$\partial_{2x} f_2^k = (7f_3^k - 8f_2^k - f_1^k)/2h^2 - (\partial_x f_3^k + 2\,\partial_x f_2^k)/h, \tag{47}$$

$$\partial_{3x} f_2^k = 3(f_3^k - f_1^k)/h^3 - 6\,\partial_x f_2^k/h^2, \tag{48}$$

$$\partial_{4x} f_2^k = 6(-5f_3^k + 4f_2^k + f_1^k)/h^4 + 12(\partial_x f_3^k + 2\,\partial_x f_2^k)/h^3, \tag{49}$$

$$\partial_x f_1^k = \partial_x f_2^k - \partial_{2x} f_2^k h + \partial_{3x} f_2^k h^2/2 - \partial_{4x} f_2^k h^3/6. \tag{50}$$

Substituting Eqs.(47) - (49) into Eq.(50), we can determine the value of $\partial_x f_1^k$ from the values of f_n^k ($n = 1, 2, 3$) and $\partial_x f_n^k$ ($n = 2, 3$). Using the same process mentioned above, we can determine the value of $\partial_x f_N^k$ by replacing h and the subscripts { $1, 2, 3$ } for grid points in Eqs.(47) - (50) with $-h$ and { $N,\ N-1\ , N-2$ }, respectively.

Combining all above processes for the four elements of thoughts of the KOND method, { [I], [II], [III], [IV]}, and for the boundary values, i.e. using Eqs.(35) - (38), Eqs.(22) - (28), Eqs.(20) and (21) to the order of $(\Delta t)^2$, and also Eqs.(47) - (50), we find the set of the discrete solutions to the 1st derivatives { $f_n^{k+1},\ \partial_x f_n^{k+1}$ } after one time step from the state of { $f_n^k,\ \partial_x f_n^k$ }. We have shown here the 1st order KOND-P scheme. If we use the 2nd order or higher order KOND-P scheme, we would obtain more accurate and stable results to the higher derivatives of f in the parabolic equations.

§ 4. Typical Numerical Results

We show here typical numerical results by the 1st order KOND-P scheme presented in the previous section. For the comparison of the numerical accuracy, we also use the conventional explicit scheme, which is denoted by "EXPL scheme" here after. The EXPL scheme obtained from the finite-difference equation is given by $f_n^{k+1} = f_n^k + D\Delta t(f_{n+1}^k - 2f_n^k + f_{n-1}^k)/h^2$. In order to test the accuracy of the numerical results, we calculate the following case with the analytical solution; { the diffusion coefficient $D = 1$, the initial profile of $f(x) = \sin(2\pi x/\lambda)$, and the boundary condition (a) of $f_n^k = 0\ (n = 1, N)$}. Here, λ is one period length of $f(x)$. The analytical solution for this case is written as $f(t,x) = \exp[-(2\pi/\lambda)^2 t]\sin(2\pi x/\lambda)$. When we define M as the number of meshes in one period length, λ is given by $\lambda = Mh$, and $M+1$ grid points cover one period length. In order to measure quantitatively the numerical accuracy, we use the root mean square deviation, σ, from the analytical solution, which is defined by

$$\sigma = \{ \frac{1}{N} \sum_{n=1}^{N} [f(t_k, x_n) - f_n^k]^2 \}^{1/2}. \qquad (51)$$

The double precision programme is used for the following numerical calculations.

Figure 1 shows typical results of computation for the time evolution of σ in the case of $M = 20$ and $D\Delta t/h^2 = 0.1$, where two lines of σ by the EXPL scheme (the mark □) and the KOND-P scheme (the mark ■) are shown in a semi-log scale. We recognize from Fig.1 that the error of the KOND-P scheme measured by σ is less than that of the EXPL scheme by about 2 orders in this case. It is also seen from Fig.1 that the rate of increment of σ in the KOND-P scheme is less than that in the EXPL scheme.

Figure 2 shows typical results of computation to see the dependence of σ on the number of meshes M in one period length in the case of $D\Delta t/h^2 = 0.1$, where two lines of σ at the time of $t = 1.0$ by the EXPL scheme (the mark □) and the KOND-P scheme (the mark ■) are shown in a semi-log scale. It is recognized from Fig.2 that higher improvement rate of accuracy by increasing the number of meshes M can be achieved in the KOND-P scheme than in the EXPL scheme. In the case of $M = 40$, the error of the KOND-P scheme measured by σ becomes less than that of the EXPL scheme by about 3 orders, as is seen in Fig.2. The data in Fig.2 also shows that improvement of accuracy by increasing the number of meshes saturates faster in the EXPL scheme than in the KOND-P scheme.

It is clearly demonstrated by the numerical results in Figs.1 and 2 that quite high accuracy can be attained by the present 1st order KOND-P scheme. The local multisubscales and delta function (LMS-DF) method reported in Ref.15 to improve numerical schemes is also applicable to the present KOND-P scheme as well as to the KOND-H scheme[12)] for the hyperbolic equation to attain further less numerical error.

§ 5. Discussion and Summary

We have presented the KOND-P scheme in detail and have shown the typical numerical results by the scheme in the previous sections. We have clarified by the numerical results that quite high accuracy can be attained by the present 1st order KOND-P scheme. The KOND-P scheme is another example of application of the KOND method to the parabolic type equations in addition to the example of the KOND-H scheme for the hyperbolic ones.[12)] The KOND method was deduced from the thought analysis on numerical schemes, which is presented briefly in § 2 to show the reason why the KOND method yields the high accuracy of the numerical results. The first two thought elements, [I] and [II], in the main set of thoughts of the KOND method, Eq.(14), require that we should solve the given equations as analytically as possible in order to attain higher accuracy, avoiding to use the finite-difference equations which already contain finite errors. The third thought element, [III], in the KOND method reveals that the set of discrete values $\{ f_n,\ \partial_i f_n,\ \partial_{ij} f_n,\ \cdots \}$ is one of the best discretization for the continuous solutions and/or the given function, which we have called "the kernel optimum discretization" of a function by the coefficients of the Taylor expansion at every grid point. The fourth thought element, [IV], in the KOND method clarifies the meaning of using the connection relations { Eqs.(8), (9), (10), $\cdots$ }, i.e. we recover approximately the lost informations included in the rest infinite terms of the Taylor expansions by the additional Taylor coefficients, which we have called "Folding of rest terms of the Taylor expansion by the connection relations". Using the two thought elements, [III] and [IV], in the KOND method, one of the authors (Y. K.) proposed a method in Ref.12 for the digital signal processing by the kernel optimum discretization for the analog signal $f(t)$ with very high frequency components. The plural applications of the KOND method, like the examples of the KOND-H scheme, the KOND-P scheme, and the method for the digital signal processing mentioned above, are themselves demonstrations showing the usefulness of "the thought analysis" introduced by one of the authors (Y. K.) to improve the objects being studied and/or to find some other new thoughts which involve generality.[12–14]

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Figure captions

Fig.1. Typical results of computation for the time evolution of numerical error measured by σ in the case of $M = 20$ and $D\Delta t/h^2 = 0.1$. Two lines of σ by the EXPL scheme (the mark □) and the KOND-P scheme (the mark ■) are shown in a semi-log scale.

Fig.2. Dependence of numerical error measured by σ on the number of meshes M in one period length in the case of $D\Delta t/h^2 = 0.1$. Two lines of σ at the time of $t = 1.0$ by the EXPL scheme (the mark □) and the KOND-P scheme (the mark ■) are shown in a semi-log scale.

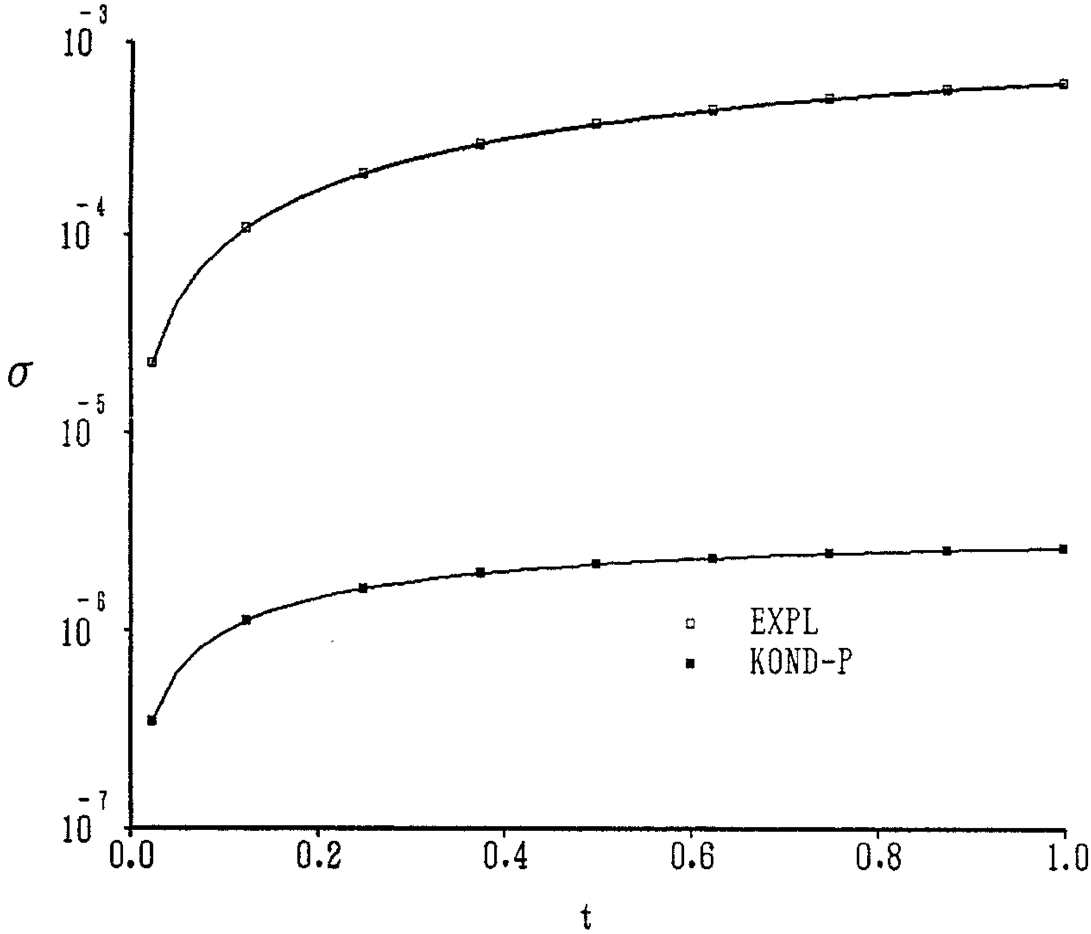

Fig.1

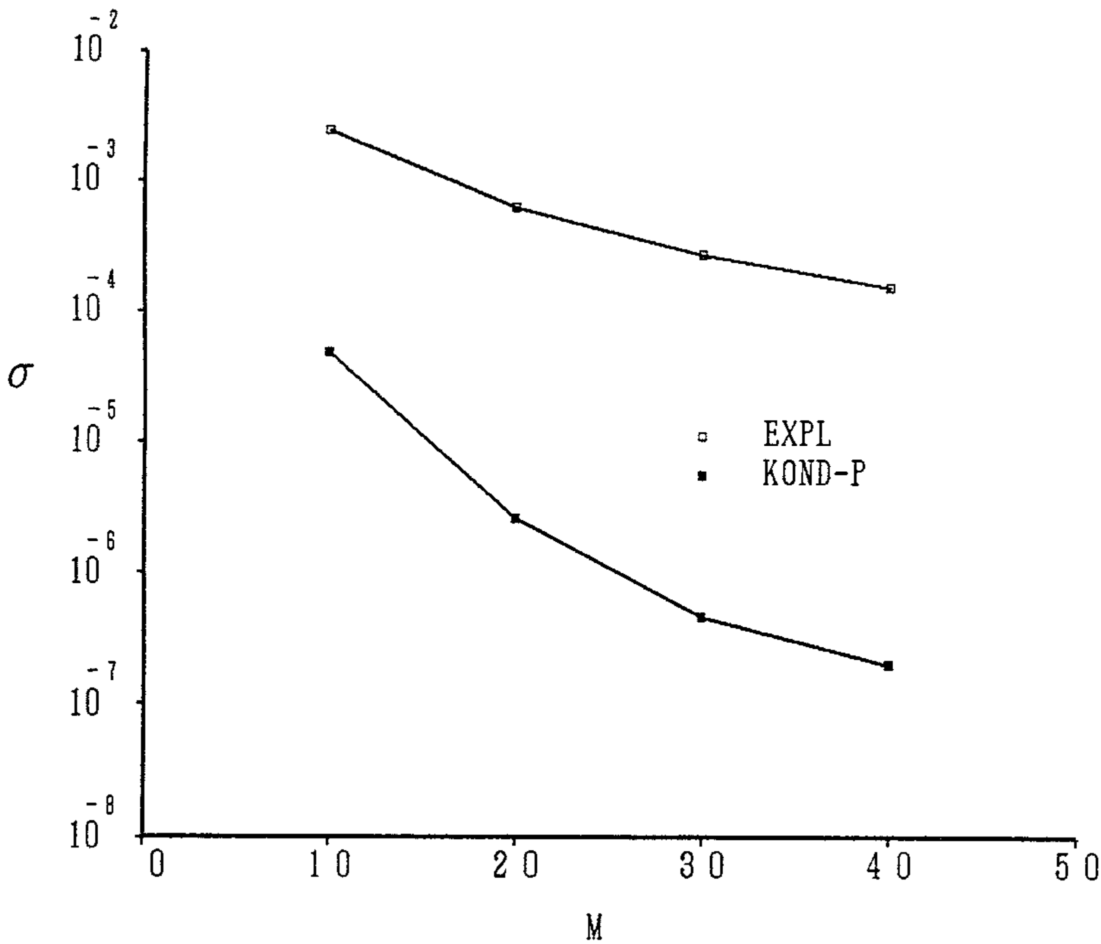

Fig.2

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