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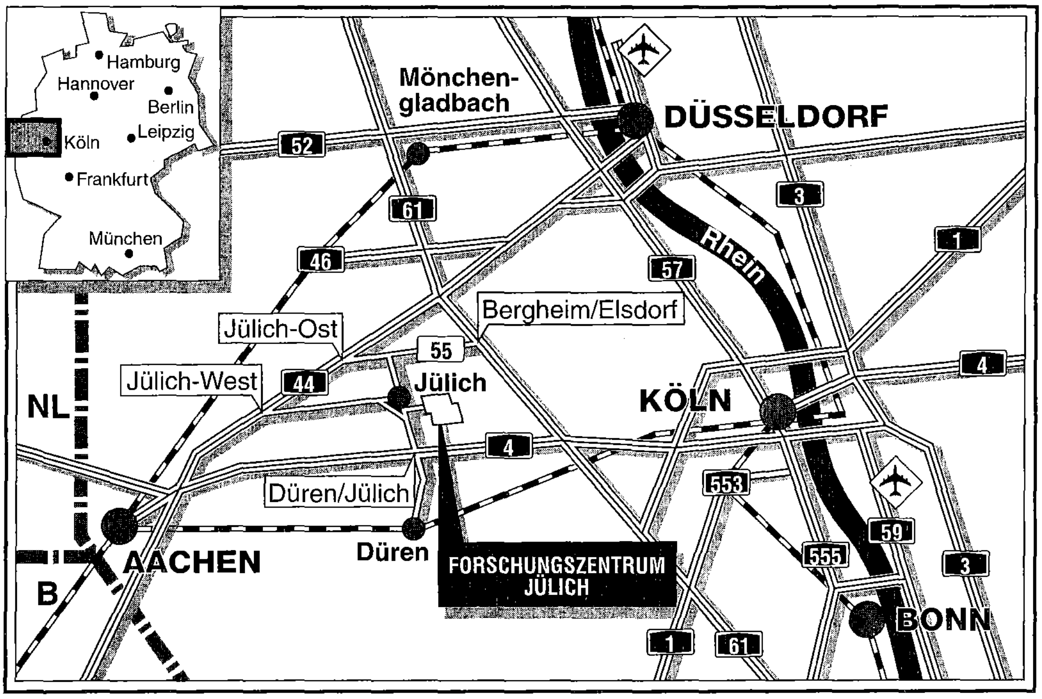

Berichte des Forschungszentrums Jülich ; 3208

ISSN 0944-2952
Institut für Plasmaphysik Jül-3208
Association EURATOM-KFA

Zu beziehen durch: Forschungszentrum Jülich GmbH · Zentralbibliothek
D-52425 Jülich · Bundesrepublik Deutschland
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Abstract

A new method to treat numerically the boundary value problem to ordinary differential equations of second order is proposed. It uses analytical solutions to the linear differential equations with constant coefficients and allows to reduce significantly the number of operations required. Comparison with the method of factorization often applied to the problem in question is done.

1. Introduction

Numerical solution of ordinary differential equations of second order (ODESO) are of importance for various applications. In particular, one deals with such equations considering transport of particles and energy in one-dimensional steady-state systems where flows are defined as:

$$J = -D \cdot \frac{d\Phi}{dx} + V \cdot \Phi. \tag{1}$$

Here Φ denotes the quantity in question e.g. particle density and D and V are the coefficient of diffusion and velocity of convection, respectively. In the case of non-stationary, two- or three-dimensional systems one can reduce transport equations to ODESO by replacement of derivatives with respect to time and certain co-ordinates by finite differences.

Methods of numerical solution of ODESO are diverse. The best choice depends on the particular situation and on the type of the boundary conditions. In the case where both conditions are imposed at the same edge the Runge-Kutta method [1] is often used. For the case with boundary conditions at both edges, which will be discussed henceforth, the method of factorization has been developed (see [2] and Appendix). This takes into account the particular features of ODESO and allows to find the solution of a linear equation by a single loop over grid knots only.

However, the following example will demonstrate that not in all cases the method of factorization is optimal. Let us consider the continuity equations for ions of different charges Z used to describe the transport of impurities in the confined zone of tokamaks [3]:

$$\frac{\partial n_z}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}(rJ_z) = -\frac{n_z}{\tau_z} + S_z. \tag{2}$$

Here t is time, r is the minor radius labeling the magnetic surfaces, $0 \leq r \leq a$, n_z and τ_z are the density of Z-ions and characteristic time of their destruction in collisions with neutral and plasma particles, S_z is the density of the ion source due to ionization of ions of the charge Z-1.

We consider a steady-state situation assuming J_z in the form (1) with D independent of r and V=0. If Z is not too high the ions in question are localized at the plasma edge in the region of a width significantly smaller than a [3]. In such a case cartesian co-ordinates can be applied and we introduce the distance from the plasma boundary, x=a-r, as such a co-ordinate. The absence of Z-ions in the plasma core is expressed by the boundary condition $n_z(x=\infty)=0$. The second boundary condition describes prompt neutralization of ions on material surfaces outside the plasma: $n_z(x=0)=0$. Additionally, we assume a simple distribution of the ion source: $S_z=S_0 \cdot \exp(-x/l_0)$, which reflects decay of the density of (Z-1)-

ions toward the plasma core. Under the above assumptions Eq.(2) has an analytical solution:

$$n_z = \frac{S_0 l_0^2}{D} \frac{l_z^2}{l_z^2 - l_0^2} [\exp(-\frac{x}{l_z}) - \exp(-\frac{x}{l_0})], \tag{3}$$

with $l_z = (D \cdot \tau_z)^{1/2}$.

It can be seen from (3) that for a numerical solution of Eq.(2) e.g. by the method of factorization with a sufficient accuracy the grid increment should be significantly smaller than l_0 and l_z. Usually $l_{0,z}$ are much smaller than the whole computation domain and the number of numerical operations can be huge even in cases where a simple exact analytical solution exists.

The above example supports the idea that dividing the computation region into intervals, in which the coefficients of the ODESO change weakly only, and using known analytical solutions in each of them, we can reduce the number of operations required. This idea underlies the method of ODESO solution proposed in the present paper.

2. Basic relationships

We start from the following standard form of ODESO:

$$\frac{d^2 y}{dx^2} + a(x) \frac{dy}{dx} + b(x) y = f(x), \tag{4}$$

with boundary conditions:

$$\sigma_{1,n} \cdot y(x_{1,n}) + \phi_{1,n} \cdot \frac{dy}{dx}(x_{1,n}) = \psi_{1,n}, \tag{5}$$

where $x_{1,n}$ corresponds to the two edges of the computation region.

The grid size is chosen such that for each interval the coefficients a and b are constant within a required accuracy if $x_i < x < x_{i+1} = x_i + \Delta x$ $(1 \leq i \leq n-1)$. The function f changes in each such interval in a "simple way", it either increases or decreases monotonically. This behaviour is approximated as follows:

$$f(x) = C_i \exp[\lambda_0 (x_i - x)] + D_i \exp[\lambda_0 (x - x_{i+1})], \tag{6}$$

where

$$\lambda_0 = \frac{1}{\Delta x} \ln \frac{f_i}{f_{i+1}}, \; C_i = f_i, \; D_i = 0, \tag{7}$$

if $f_i = f(x_i)$ and $f_{i+1} = f(x_{i+1})$ have the same sign and

$$\lambda_0=\frac{1}{\Delta x},\ C_i=\frac{f_m-e^{-1}f_{m+1}}{1-e^{-2}},\ D_i=\frac{f_{m+1}-e^{-1}f_m}{1-e^{-2}}, \tag{8}$$

in the opposite case. Another approximation of f(x), e.g. by harmonic functions, can also be used depending on the physical situation.

For constant a and b and f in the form (6) the solution to Eq.(4) within the interval $x_i<x<x_{i+1}$ is:

$$y_i=G_is_i(x)+H_it_i(x)+E_ip_i(x)+F_ir_i(x). \tag{9}$$

The first two terms in (9) with

$$G_i=\frac{C_i}{\lambda_0^2+a\lambda_0+b},\ H_i=\frac{D_i}{\lambda_0^2+a\lambda_0+b}, \tag{10}$$

$$s_i(x)=\exp[\lambda_0(x_i-x)],\ t_i(x)=\exp[\lambda_0(x-x_{i+1})], \tag{11}$$

correspond to a partial solution, the functions p(x) and r(x) are solutions with $f\equiv0$ and E_i and F_i are arbitrary coefficients so far. The form of the functions p and r is determined by the sign of the determinant $\Delta=a_i^2-4b_i$ [4]:

$$p_i(x)=\exp[-\lambda_+(x-x_i)],\ r_i(x)=\exp[\lambda_-(x_{i+1}-x)] \tag{12}$$

with $\lambda_\pm=(-a_i\pm\Delta^{1/2})/2$ for $\Delta>0$,

$$p_i(x)=\exp[-\frac{a}{2}(x-x_i)](x-x_i),\ r_i(x)=\exp[\frac{a}{2}(x_{i+1}-x)](x_{i+1}-x) \tag{13}$$

for $\Delta=0$ and

$$p_i(x)=\exp[-\frac{a}{2}(x-x_i)]\sin[\sqrt{-\Delta}\,(x-x_i)], \tag{14}$$

$$r_i(x)=\exp[\frac{a}{2}(x_{i+1}-x)]\sin[\sqrt{-\Delta}\,(x_{i+1}-x)] \tag{15}$$

for $\Delta<0$.

For the derivative of y_i we have:

$$\frac{dy_i}{dx}=G_iw_i(x)+H_iz_i(x)+E_iu_i(x)+F_iv_i(x), \tag{16}$$

where $u_i(x)$, $v_i(x)$, $w_i(x)$, $z_i(x)$ are derivatives of the functions $p_i(x)$, $r_i(x)$, $s_i(x)$ and $t_i(x)$, respectively.

The coefficients E_i and F_i are determined from a system of 2(n-1) linear equations. These follow from the requirement of continuity of y_i and dy_i/dx at the grid knots: $y_i(x_{i+1})=y_{i+1}(x_{i+1})$ and $dy_i/dx(x_{i+1})=dy_{i+1}/dx(x_{i+1})$ for $i=1,\ldots,n-2$ - and from the boundary conditions (5). The structure of the equations - each of which includes only 4 unknown quantities E_i, E_{i+1}, F_i and F_{i+1} - makes its possible to solve them without evaluation of large determinants. Thus one obtains the following recurrent relationships:

$$E_i=\delta_i+\xi_i F_i,\ F_i=\theta_i+\varrho_i E_{i+1}+\gamma_i F_{i+1}, \tag{17}$$

with

$$\delta_{i+1}=\frac{G_i w_{i,2}+H_i z_{i,2}-G_{i+1}w_{i+1,1}-H_{i+1}z_{i+1,1}+\delta_i u_{i,2}+\theta_i(\xi_i u_{i,2}+v_{i,2})}{u_{i+1,1}-\varrho_i(\xi_i u_{i,2}+v_{i,2})}, \tag{18}$$

$$\xi_{i+1}=\frac{\gamma_i(\xi_i u_{i,2}+v_{i,2})-v_{i+1,1}}{u_{i+1,1}-\varrho_i(\xi_i u_{i,2}+v_{i,2})}, \tag{19}$$

where

$$\theta_k=\frac{G_{k+1}s_{k+1,1}+H_{k+1}t_{k+1,1}-G_k s_{k,2}-H_k t_{k,2}-\delta_k P_{k,2}}{d_0},\rho_k=\frac{P_{k+1,1}}{d_0},\gamma_k=\frac{r_{k+1,1}}{d_0},$$

$p_{i,1}=p_i(x_i)$, $p_{i,2}=p_i(x_{i+1})$ and analogously for functions r, s, t, u, v, w and z, $d_0=r_{k,2}+\xi_k P_{k,2}$

The coefficients ξ_1 and δ_1 are found from the boundary conditions at $x=x_1$:

$$\delta_1=\frac{\psi_1-\sigma_1(G_1 s_{1,1}+H_1 t_{1,1})-\phi_1(G_1 w_{1,1}+H_1 z_{1,1})}{\sigma_1 p_{1,1}+\phi_1 u_{1,1}}, \tag{20}$$

$$\xi_1=-\frac{\sigma_1 r_{1,1}+\phi_1 v_{1,1}}{\sigma_1 p_{1,1}+\phi_1 u_{1,1}}, \tag{21}$$

The coefficient F_{n-1} is obtained from the boundary conditions at $x=x_n$:

$$F_{n-1}=\frac{\bar{\delta}-\delta_{n-1}}{\xi_{n-1}-\bar{\xi}}, \tag{22}$$

where

$$\bar{\delta}=\frac{\psi_n-\sigma_n(G_{n-1}s_{n-1,2}+H_{n-1}t_{n-1,2})-\phi_n(G_{n-1}w_{n-1,2}+H_{n-1}z_{n-1,2})}{\sigma_2 p_{n-1,2}+\phi_n u_{n-1,2}}, \tag{23}$$

$$\bar{\xi}=-\frac{\sigma_2 r_{n,2}+\phi_2 v_{n,2}}{\sigma_2 p_{n,2}+\phi_2 u_{n,2}}, \tag{24}$$

The coefficient E_{n-1} is calculated from the first of relations (17).

3. Numerical example and comparison with the method of factorization

As an example for applicability of the method proposed above we have computed the solution of the equation:

$$\frac{d^2y}{dx^2} + 10x\frac{dy}{dx} = 50x^2y - \exp(-300x^2), \tag{26}$$

on the interval $0 \le x \le 1$ with boundary conditions $y(0)=0$ and $dy/dx(1)=0$ (see Fig.1a). Fig.1b shows the solutions of the same equation obtained by the method of factorization. Different curves correspond to solutions found for different grid sizes.

Solutions found by the two different methods are practically the same for the maximal $n=501$ considered here and this is an evidence that they both are close to the "exact" one. On the other hand the difference between solutions obtained with smaller n is obvious. Our method gives a qualitatively correct approximation to the "exact" solution already for the smallest $n=11$. For $n=31$ the error does not exceed 5% anywhere. In the case of solutions obtained by the method of factorization the one with $n=11$ must be classified as qualitatively wrong and even for $n=31$ the error still remains unacceptable in the region close to $x=0$.

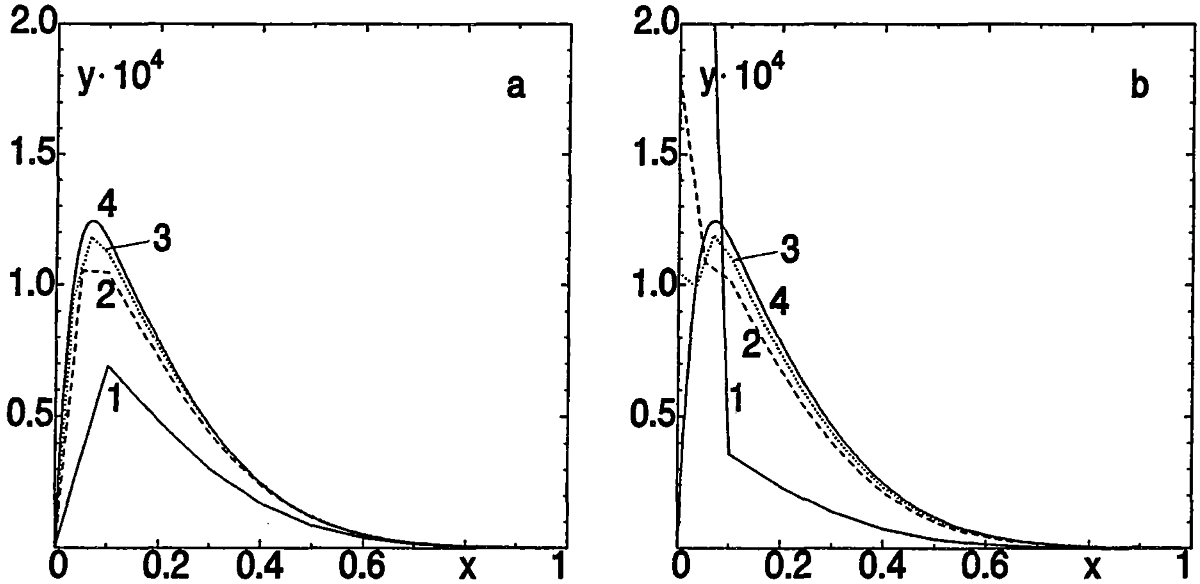

Figure 1. Numerical solutions of the Eq.(25) found by the method proposed in the present paper (a) and by the method of factorization for different numbers of steps: 1. n=11, 2. n=21, 3. n=31 and 4. n=501.

4. Conclusion

A new method of numerical solution of the boundary value problem to linear ordinary differential equation of second order is proposed. It is based on utilization of exact analytical solutions to equations with constant coefficients and a specified form of the right hand side. For a small number of the grid steps this method gives a significantly better approximation to the "exact" solution than the method of factorization. The method proposed here can directly be applied to cases with variable length of the grid increment.

As a disadvantage of the method one could consider that it can not be generalized in a straightforward way for a system of ODESO. However for the vast majority of applications one has to deal with non-linear equations which are solved iteratively. Hence application of methods developed especially to solve systems of linear equations does not provide any improved numerical performance in general. In this case each of the equations can be solved by the proposed method separately in loops or in parallel. Such a procedure has been employed in the code RITM (Radiation from Impurities in a Transport Model) [3], [5]. This code models self-consistently the transport of background plasma and impurities coupled through radiation and dilution. Depending on the cases studied up to fifty transport equations are solved simultaneously by the method proposed above. Skilful mixing of iterations makes it possible to obtain converged solutions describing even such highly non-linear situations as "detached plasma" in limiter tokamaks [3].

Appendix: method of factorization

Using the approximation $dy/dx \approx (y_{i+1}-y_i)/h$ with the increment h independent of x one obtains, instead of Eq.(4), the following system of linear algebraic equations:

$$\frac{y_{i+1}-2y_i+y_{i-1}}{h^2}+a_i\frac{y_{i+1}-y_{i-1}}{2h}=b_iy_i-f_i, \tag{27}$$

or

$$y_{i+1}+m_iy_i+n_iy_{i-1}=\bar{f}h^2, \tag{28}$$

with

$$m_i=-\frac{4+2b_ih^2}{2+a_ih},\ n_i=\frac{2-a_ih}{2+a_ih},\ \bar{f}_i=-\frac{2f_i}{2+a_ih}. \tag{29}$$

Let us assume that using the whole system of equations (27) we have excluded y_{i-1} from Eq.(26) and resolved it respect to y_i. The result can be written as follows:

$$y_i = c_i(d_i-y_{i+1}), \tag{30}$$

where c_i and d_i are certain unknown coefficients. Analogously we have

$$y_{i-1} = c_{i-1}(d_{i-1}-y_i). \tag{31}$$

Substituting this into Eq.(27) and resolving it respect to y_i one obtains:

$$y_i = \frac{(\mathcal{f}_i h^2 - n_i c_{i-1} d_{i-1}) - y_{i+1}}{m_i - n_i c_{i-1}}. \tag{32}$$

Comparing of Eqs.(29) and (31) we find the recurrent relationships:

$$c_i = (m_i - n_i c_{i-1})^{-1},\ d_i = \mathcal{f}_i h^2 - n_i c_{i-1} d_{i-1}. \tag{33}$$

The values c_1 and d_1 are obtained from the comparison of Eq.(27) and the relationship between y_1 and y_2 which follows from the boundary condition at $x=x_1$:

$$c_1 = \frac{\phi_1}{\sigma_1 h - \phi_1},\ d_1 = \frac{\psi_1 h}{\phi_1}. \tag{34}$$

To calculate y_i according to Eq.(31) one needs to know y_n. This is found from the boundary condition at $x=x_2$ and Eq.(29) for i=n-1:

$$y_n = \frac{\psi_2 h + \phi_2 c_{n-1} d_{n-1}}{\sigma_2 h + \phi_2 (c_{n-1}+1)}. \tag{35}$$

Acknowledgements

The author is grateful to H.Gerhauser, A.Kaleck and D.Reiter for helpful discussions of the manuscript.

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FORSCHUNGSZENTRUM JÜLICH GmbH

Jül-3208
March 1996
ISSN 0944-2952