Rate of Convergence and Stability of a Numerical Algorithm for Neutrons Transport Equation

NIKOS MASTORAKIS
Head of the Department of Computer Science
Military Inst. of University Education / Hellenic Naval Academy
Terma Hatzikyriakou 18539,
Piraeus, GREECE
http://www.wseas.org/mastorakis

OLGA MARTIN
Department of Mathematics
University "Politehnica" of Bucharest
Splaiul Independentei 313
Bucharest, ROMANIA

Abstract: - This paper describes a numerical procedure to solve the homogeneous boundary problem for a stationary transport equation. We prove that the finite differences scheme based on the integral identity method is stably and convergent. The error value that corresponds to the numerical solution is obtained using the Lax theorem.

Key-Words: integral-differential equation, finite differences scheme, integral identity method.

1 Introduction

The growth of the computer technology has led to the development of numerical algorithms for solving the mathematical physics problems. Naturally, this has raised fundamental questions about the convergence and the stability of these algorithms. An instable scheme will be sensitive to the rounded errors that appear in the calculating process and thus, the numerical solution will differ from the exact solution.

There is a large literature on the numerical solution of a neutrons transport equation, [1],[5],[6],[8],[11], [13]. The recent studies use the methods of Ritz and Galerkin, the method of least squares, the method of finite elements and Nyström method.

The algorithm proposed by us in the work, replaces the solution of an integral-differential equation with homogeneous boundary conditions by the solution of a diffusion equation with non-homogeneous boundary conditions. For this new problem we study the stability and the convergence rate of a differences scheme based on the integral identity method.

2 Problem formulation

In the stationary case, we consider a transport equation of the form

$$\mu \frac{\partial \varphi(x,\mu)}{\partial x} + \varphi(x,\mu) = \frac{1}{\alpha} \int_{-1}^{1} \varphi(x,\mu')d\mu' + f(x,\mu) \tag{1}$$

where

$$\alpha > 0,\ \forall (x,\mu) \in D_1 \times D_2 = [0,H] \times [-1,1],$$
$$D_2 = D_2' \cup D_2'' = [-1,0] \cup [0,1].$$

The boundary conditions are

$$\begin{aligned} &\varphi(0,\mu) = 0 \text{ if } \mu > 0 \\ &\varphi(H,\mu) = 0 \text{ if } \mu < 0 \end{aligned} \tag{2}$$

Here φ is the density of neutrons, which migrate in a direction defined by the angle γ against Ox axis and we denote $\mu = \cos\gamma$. Let us consider the radioactive source f as a even function with respect μ.
Using the notations:

$$\varphi^+ = \varphi(x,\mu) \text{ if } \mu > 0; \quad \varphi^- = \varphi(x,\mu) \text{ if } \mu < 0 \tag{3}$$

and substituting $\mu'' = -\mu'$, we get

$$\int_{-1}^{0} \varphi(x,\mu')d\mu' = \int_{0}^{1} \varphi(x,-\mu'')d\mu'' = \int_{0}^{1} \varphi^- d\mu''.$$

Then the conditions (2) become

$$\varphi^+(0,\mu) = 0, \; \varphi^-(H,\mu) = 0 \tag{4}$$

and the equation (1) can be rewritten in the form

$$\begin{aligned} &\mu\frac{\partial\varphi^+}{\partial x} + \varphi^+ = \frac{1}{\alpha}\int_0^1 (\varphi^+ + \varphi^-)d\mu' + f^+ \\ &-\mu\frac{\partial\varphi^-}{\partial x} + \varphi^- = \frac{1}{\alpha}\int_0^1 (\varphi^+ + \varphi^-)d\mu' + f^- \end{aligned} \tag{5}$$

Adding and subtracting the equations (5) and introducing the notations:

$$\begin{aligned} &u = \frac{1}{2}\left(\varphi^+ + \varphi^-\right), \; v = \frac{1}{2}\left(\varphi^+ - \varphi^-\right) \\ &g = \frac{1}{2}\left(f^+ + f^-\right), \; r = \frac{1}{2}\left(f^+ - f^-\right) = 0 \end{aligned} \tag{6}$$

we obtain the following system

$$\begin{aligned} &\mu\frac{\partial v}{\partial x} + u = \frac{2}{\alpha}\int_0^1 u\,d\mu + g \qquad (a) \\ &\mu\frac{\partial u}{\partial x} + v = 0 \qquad (b) \end{aligned} \tag{7}$$

The boundary conditions become

$$\begin{aligned} &u + v = 0 \quad \text{for } x = 0, \\ &u - v = 0 \quad \text{for } x = H. \end{aligned} \tag{8}$$

Now, we find v from the second equation of (7) and using the first equation, we rewrite the problem (7)-(8) in the following form

$$-\mu^2\frac{\partial^2 u}{\partial x^2} + u = \frac{2}{\alpha}\int_0^1 u\,d\mu + g \tag{9}$$

$$\left.\left(u - \mu\frac{\partial u}{\partial x}\right)\right|_{x=0} = \left.\left(u + \mu\frac{\partial u}{\partial x}\right)\right|_{x=H} = 0 \tag{10}$$

In order to get a solution of the problem (9)-(10), we consider on x axis two points systems:

- a principal system: $\{x_k\} = \Delta_1'$, $k\in\{0, 1,\ldots,N\}$, with $x_0 = 0$, $x_N = H$ and $h = x_{k+1} - x_k$;
- a secondary system, $\{x_{k+1/2}\} = \Delta_1''$, $k \in \{0,1,2,\ldots, N-1\}$, which verifies the inequalities: $x_{k-1/2} < x_k < x_{k+1/2}$, where

$$x_{k+1/2} = (x_k + x_{k+1})/2$$

and

$$0 = x_0 < x_{1/2} < \ldots < x_{N-1/2} < x_N = H.$$

Besides, let $\Delta_2 = \{\mu_l\}, l \in \{0,1,\ldots,L\}$ be a partition of the interval $D_2'' = [0,1]$ and $\tau = \mu_{l+1} - \mu_l$, $l \in \{0,1,\ldots,L-1\}$.
Further on, we consider $H = 1$. For every value $\mu_l \in \Delta_2$, the problem (9)-(10) becomes:

$$-\mu_l^2\frac{d^2u(x,\mu_l)}{dx^2} + u(x,\mu_l) = F(x,\mu_l) \tag{11}$$

where

$$F(x,\mu_l) = S(x) + g(x,\mu_l), \; S(x) = \frac{2}{\alpha}\int_0^1 u(x,\mu)d\mu$$

and

$$\begin{aligned} &\left.\left(u(x,\mu_l) - \mu_l\frac{du(x,\mu_l)}{dx}\right)\right|_{x=0} = 0 \\ &\left.\left(u(x,\mu_l) + \mu_l\frac{du(x,\mu_l)}{dx}\right)\right|_{x=1} = 0 \end{aligned} \tag{12}$$

Now (11)-(12) is a boundary problem for a one-dimensional diffusion equation (11). Integrating (11) with respect to x on the intervals: $(x_{k-1/2}, x_{k+1/2})$, we obtain

$$-J_{k+1/2} + J_{k-1/2} + \int_{x_{k-1/2}}^{x_{k+1/2}} (u - F)dx = 0 \tag{14}$$

where

$$J_{k\pm1/2} = J(x_{k\pm1/2}),\quad J(x,\mu_l) = \mu_l^2\,\frac{du(x,\mu_l)}{dx}.$$

We find $J_{k-1/2}$ integrating (11) on the interval $(x_{k-1/2}, x)$, where $x\in(x_{k-1}, x_k)$. We get

$$\mu_l^2\,\frac{du(x,\mu_l)}{dx} = J_{k-1/2} + \int_{x_{k-1/2}}^{x}(u-F)dx \tag{15}$$

Then, dividing (15) by μ_l^2 and integrating on (x_{k-1}, x_k) we have

$$u_k - u_{k-1} = J_{k-1/2}\int_{x_{k-1}}^{x_k}\frac{dx}{\mu_l^2} + \int_{x_{k-1}}^{x_k}\frac{dx}{\mu_l^2}\int_{x_{k-1/2}}^{x}(u-F)d\xi \tag{16}$$

where $u_k = u(x_k, \mu_l)$. Finally, we get

$$J_{k-1/2} = \frac{\mu_l^2}{h}\left[u_k - u_{k-1} - \frac{1}{\mu_l^2}\int_{x_{k-1}}^{x_k}dx\int_{x_{k-1/2}}^{x}(u-F)d\xi\right] \tag{17}$$

In a similar manner, we obtain the exact relation for $J_{k+1/2}$ replacing k by k+1. Consequently, the equality (14) becomes:

$$\mu_l^2\left(\frac{u_k-u_{k+1}}{h} + \frac{u_k-u_{k-1}}{h}\right) + \int_{x_{k-1/2}}^{x_{k+1/2}}(u-F)d\xi =$$
$$= -\frac{1}{h}\int_{x_k}^{x_{k+1}}dx\int_{x_{k+1/2}}^{x}(u-F)d\xi + \frac{1}{h}\int_{x_{k-1}}^{x_k}dx\int_{x_{k-1/2}}^{x}(u-F)d\xi$$

where $k\in\{1,2,\ldots,N\text{-}1\}$. (18)

The formula (16) is named the fundamental identity for the finite differences equations.

Let us now define the operator A on the set U of the solutions of equation (11) that satisfy the boundary conditions (12)

$$(Au)_k = -\frac{\mu_l^2}{\Delta x_k}\left(\frac{u_{k+1}-u_k}{h} - \frac{u_k-u_{k-1}}{h}\right) + \int_{x_{k-1/2}}^{x_{k+1/2}}udx$$
$$+\frac{1}{\Delta x_k}\left[\frac{1}{h}\cdot\int_{x_k}^{x_{k+1}}dx\int_{x_{k+1/2}}^{x}ud\xi - \frac{1}{h}\cdot\int_{x_{k-1}}^{x_k}dx\int_{x_{k-1/2}}^{x}ud\xi\right] \tag{19}$$

$$(F)_k = \frac{1}{\Delta x_k}\int_{x_{k-1/2}}^{x_{k+1/2}}Fdx +$$
$$+\frac{1}{\Delta x_k}\left[\frac{1}{h}\int_{x_k}^{x_{k+1}}dx\int_{x_{k+1/2}}^{x}Fd\xi - \frac{1}{h}\int_{x_{k-1}}^{x_k}dx\int_{x_{k-1/2}}^{x}Fd\xi\right]$$

where
$\Delta x_k = x_{k+1/2} - x_{k-1/2} = h,\quad k\in\{1,2,\ldots,n-1\}.$

Writing now (18) for k = 1, 2,…, n –1, we get the system

$$Au = F \tag{20}$$

To study the approximations of the equation (20), we consider the space Φ of the reticulated functions

$$u^h = (u_0^h, u_1^h, u_2^h, \ldots, u_{n-1}^h, u_n^h)$$

that are defined in the points $x_0, x_1,\ldots,x_n$.
In order to can use the functions F and u, which can to have the discontinuous points in any points x_i that belong to the principal system, we define the value of the function in the node x_k of the form

$$(F^h)_k = \frac{1}{\Delta x_k}\int_{x_{k-1/2}}^{x_{k+1/2}}Fdx = \frac{1}{h}\int_{x_{k-1/2}}^{x_{k+1/2}}Fdx \tag{21}$$

if the step is constant. In the following, we write the approximate form of the equation (20)

$$A^h u^h = F^h \tag{22}$$

Where

$$(A^h u^h)_k = -\frac{\mu_l^2}{\Delta x_k}\left(\frac{u_{k+1}-u_k}{h} - \frac{u_k-u_{k-1}}{h}\right) +$$
$$+\frac{1}{\Delta x_k}u_k h = -\frac{\mu_l^2}{\Delta x_k}\left(\frac{u_{k+1}-u_k}{h} - \frac{u_k-u_{k-1}}{h} - \frac{u_k h}{\mu_l^2}\right)$$

k = 1, 2,…,n-1 and $\Delta x_k = h$. (23)

Let us now consider in Φ the scalar product of the form

$$(a,b) = \sum_{k=1}^{n-1}\Delta x_k a_k b_k \tag{24}$$

and the norm

$$\|a\|^2 = \sum_{k=1}^{n-1}\Delta x_k a_k^2 \tag{25}$$

3 Stability and convergence

Let us now show that the difference scheme is stably. We suppose that $F \in Q^2([0,1])$ (the function and its derivates until two order are continuous everywhere in [0,1] except a finite number of first-order discontinuous that belong to the set $\{x_1,\ldots,x_n\}$) and approximate solution of equation (23), $u^h \in \Phi$ is continuous on [0, 1].
Using the finite differences method, the boundary conditions (12) become

$$u_0 = \mu_l \frac{u_1 - u_0}{h} \Rightarrow u_0 = \frac{\mu_l}{h + \mu_l} u_1 \tag{26}$$

$$u_n = -\mu_l \frac{u_n - u_{n-1}}{h} \Rightarrow u_n = \frac{\mu_l}{h + \mu_l} u_{n-1} \tag{27}$$

By using (24), (26) and (27), we get

$$(u^h, F^h) = (u^h, A^h u^h) =$$

$$= -\mu_l^2 \sum_{k=1}^{n-1} \left(\frac{u_{k+1} - u_k}{h} - \frac{u_k - u_{k-1}}{h} \right) \cdot u_k + \sum_{k=1}^{n-1} u_k^2 \cdot h =$$

$$= \mu_l^2 \sum_{k=2}^{n-1} \frac{(u_k - u_{k-1})^2}{h} + \sum_{k=1}^{n-1} u_k^2 \cdot h + \tag{28}$$

$$+ \mu_l^2 \frac{u_1(u_1 - u_0)}{h} + \mu_l^2 \frac{u_{n-1}(u_{n-1} - u_n)}{h} =$$

$$= \mu_l^2 \sum_{k=2}^{n-1} \frac{(u_k - u_{k-1})^2}{h} + \frac{\mu_l^2}{\mu_l + h}\left(u_1^2 + u_{n-1}^2\right) + \|u\|^2 \geq \|u\|^2$$

It should observe that this result doesn't lead to the relation between u^h and g, which defines the stability of our difference scheme:

$$\left\|u^h\right\| \leq C_1 \left\|g^h\right\| \tag{29}$$

where C_1 is an independent constant of h and g.

In view of the equation (11) we have

$$F(x, \mu_l) = S(x) + g(x, \mu_l),\ S(x) = \frac{2}{\alpha} \int_0^1 u(x, \mu) d\mu$$

Let us assume that solution of the problem (11)-(12) is of the form

$$u(x, \mu) = \mu^r \phi(x),\ r \geq 1 \tag{30}$$

In this case, [10], the following inequalities are found

$$(u^h, F^h) = \sum_{k=1}^{n-1} h u_k^h F_k^h =$$

$$= \sum_{k=1}^{n-1} h u_k^h \frac{1}{h} \int_{x_{k-1/2}}^{x_{k+1/2}} g(x, \mu_l) dx + \tag{31}$$

$$+ \sum_{k=1}^{n-1} h u_k^h \frac{2}{\alpha h} \int_{x_{k-1/2}}^{x_{k+1/2}} dx \int_0^1 u_k^h(x, \mu) d\mu =$$

$$= (u^h, g^h) + \sum_{k=1}^{n-1} h u_k^h \frac{2}{\alpha h} \int_{x_{k-1/2}}^{x_{k+1/2}} \phi(x) dx \int_0^1 \mu^r d\mu =$$

$$= (u^h, g^h) + \sum_{k=1}^{n-1} h u_k^h \frac{2}{\alpha h} \cdot \frac{1}{(r+1)\mu_l^r} \int_{x_{k-1/2}}^{x_{k+1/2}} \mu_l^r \varphi_k(x) dx =$$

$$= (u^h, g^h) + \frac{2}{(r+1)\alpha \mu_l^r} \sum_{k=1}^{n-1} h (u_k^h)^2$$

Then, using the Cauchy – Schwarz inequality

$$(a^h, b^h) \leq \left\|a^h\right\|_\Phi \cdot \left\|b^h\right\|_\Phi$$

we get

$$(u^h, F^h) \leq \left\|u^h\right\| \cdot \left\|g^h\right\| + \frac{2}{(r+1)\alpha \mu_l^r} \left\|u^h\right\|^2$$

Taking (28) into account, it can be show the following inequalities

$$\left\|u^h\right\|_\Phi \cdot \left\|g^h\right\|_\Phi + \frac{2}{(r+1)\alpha \mu r} \left\|u^h\right\|_\Phi^2 \geq \tag{32}$$

$$\geq (u^h, F^h) \geq \left\|u^h\right\|_\Phi^2 .$$

Hence

$$\left\|g^h\right\| \geq \left(1 - \frac{2}{(r+1)\alpha \mu_l^r} \right) \cdot \left\|u^h\right\| . \tag{33}$$

If $\frac{1}{\alpha} < \frac{(r+1)\mu_l^r}{2} \leq \frac{r+1}{2}$, we obtain

$$\left\|u^h\right\|_\Phi \leq C_{1l} \left\|g^h\right\|_\Phi \tag{34}$$

for every μ_l fixed into Δ_2. Finally, from the definition

$$C_1 = \max_{1 \leq l \leq L-1} C_{1l}$$

we get

$$\left\|u^h\right\|_\Phi \le C_1\|g\|_\Phi \tag{35}$$

and the stability of differences scheme is proved.

Definition

The problem

$$A^h u^h = F^h \tag{22}$$

is an approximations of *the n- order* with respect to the solution u of the equation (20), if there are the constants h_1 and M_1 such that for $h < h_1$ we have

$$\left\|A^h(u)_h - F^h\right\|_\Phi \le M_1 h^n \tag{36}$$

where $(u)_h$ is the vector with the n-1 dimension from Φ with the components $u(x_k)$. Using the equations (20) and (22) we get

$$\begin{aligned}\left\|A^h\left[(u)_h - u^h\right]\right\|_\Phi &= \left\|A^h(u)_h - F + F - F^h\right\|_\Phi \le \\ &\le \left\|A^h(u)_h - F\right\|_\Phi + \left\|F - F^h\right\|_\Phi \le \\ &\le \left\|\xi^h\right\|_\Phi + \left\|\eta^h\right\|_\Phi + \left\|\theta^h\right\|_\Phi\end{aligned}$$

where

$$(\xi^h)_k = \frac{1}{h}\left(\int_{x_{k-1/2}}^{x_{k+1/2}} u(x,\mu_l)dx - u(x_k,\mu_l)h\right)$$

$$\begin{aligned}(\eta^h)_k &= -\frac{1}{h^2}\int_{x_k}^{x_{k+1}} dx \int_{x_{k+1/2}}^{x} u(t,\mu_l)dt + \\ &+ \frac{1}{h^2}\int_{x_{k-1}}^{x_k} dx \int_{x_{k-1/2}}^{x} u(t,\mu_l)dt\end{aligned}$$

$$\begin{aligned}(\theta^h)_k &= -\frac{1}{h^2}\int_{x_k}^{x_{k+1}} dx \int_{x_{k+1/2}}^{x} F(t,\mu_l)dt + \\ &+ \frac{1}{h^2}\int_{x_{k-1}}^{x_k} dx \int_{x_{k-1/2}}^{x} F(t,\mu_l)dt\end{aligned}$$

Since the functions F and u have its derivates continuous until two order everywhere in [0,1], except a finite number of first-order discontinuous that belong to the set $\{x_1,\ldots,x_n\}$ and using the Taylor formula in the vicinity of the nodes x_k, we get

$$\left|(\xi^h)_k\right| \le N_1 h;\ \left|(\eta^h)_k\right| \le N_2 h;\ \left|(\theta^h)_k\right| \le N_3 h$$

Let us now define

$$(\omega^h)_k = \max\left(\left|(\xi^h)_k\right|, \left|(\eta^h)_k\right|, \left|(\theta^h)_k\right|\right) = Nh$$

where $N = \max(N_1, N_2, N_3)$. By using the definition (25), the square of the norm verifies the inequality

$$\left\|\omega^h\right\|_\Phi^2 = \sum_{k=1}^{n-1}(\omega^h)_k^2 h \le N^2 h^3$$

Consequently,

$$\left\|\omega^h\right\|_\Phi \le M h^{3/2} \tag{37}$$

Thus it has been show that the differences scheme (22) approximates the initial problem (20) with the order 3/2 with respect to the solution u.
With the help of the following theorem,[5], we shall estimate the speed of the convergence of the approximate solution u^h to the exact solution u.

Theorem (Lax). If

1. the differences scheme (22) approximates the initial problem (20) with the order n with respect to the solution u;
2. A^h is a linear operator;
3. the difference scheme is stably in accordance with (29), then the solution of the approximate problem is convergent to the exact solution and the evaluation of the convergent speed is defined by the following inequality

$$\left\|(u)_h - u^h\right\| \le MC_1 h^n \tag{38}$$

Using the above theorem to our problem, the value of the error is

$$\left\|(u)_h - u^h\right\|_\Phi \le 3\left\|\omega^h\right\|_\Phi C_1 \le 3C_1 M h^{3/2} = K_l h^{3/2}$$

for μ_l fixed. Let us now consider $K = \max\limits_{0\le l\le L} K_l$ and finally, the estimation of the error is the following

$$\left\|(u)_h - u^h\right\| \le K h^{3/2} \tag{39}$$

References:

[1]. Ackroyd R.T., Gashut A.M., O.A. Abuzid O., Discontinuous Variational Solutions for the Neutron Diffusion Equation, *Ann. Nucl. Energy*, **23**, (1996), 1289.

[2]. Case K. M. and Zweifel P. F., *Linear Transport Theory*, Addison-Wesley, Massachusetts, 1967.

[3]. Davis W. R., *Classical Fields, Particles and the Theory of Relativity* , Gordon and Breach, New York, 1970.

[4]. Glasstone S. and Kilton C., *The Elements of Nuclear Reactors Theory,* Van Nostrand, Toronto – New York – London, 1982.
[5]. Marchouk G., *Méthodes de Calcul Numérique*, Édition MIR de Moscou, 1980.
[6]. Marchouk G. and Shaydourov V., *Raffinement des Solutions des Schémas aux Différences*, Édition MIR de Moscou, 1983.
[7]. Marciuk G. and Lebedev V. , *Cislennie Metodî v Teorii Terenosa Neitronov,* Atomizdat, Moscova, 1971.
[8]. Martin O., Une Méthode de Résolution de l'Équation du Transfert des Neutrons*, Rev.Roum. Sci. Tech.- Méc. Appl.,* **37**,6*,* (1992), 623-646.
[9] Martin O.*,* Analytical and Numerical Solutions for One- Dimensional Transport Equation, *WSEAS Transactions on Circuits and Systems,* **3**,7(2004), 383-389.
[10] Mastorakis N., Martin O.*,* About theNumerical Solution of a Stationary Transport Equation, *WSEAS Transactions on Information Sciences & Applications,* **2**,9(2005), 1373-1380.
[11]. Mihailescu N., Oscillations in the Power Distribution in a Reactor*, Rev. Nuclear Energy,* **9,** 1-4 (1998), 37-41.
[12]. Mokhtar-Kharroubi M.*, Topics in Neutron Transport Theory,* Series on Advances in Math. For Applied Sciences, Bellomo and Brezzi, 1997.
[13]. Ntouyas S. K., *Global Existence for Neutral Functional Integral Differential Equations*, Proc. 2nd World Congress of Nonlinear Analysts, 1997, 2133-2142.
[14]. Parton V.Z., Perlin P.I., *Mathematical Methods o f the Theory of Elasticity,* MIR Publishers Moscow,1984.
[15]. Pilkuhn H., *Relativistic Particle Physics*, Springer Verlag, New York - Heidelberg-Berlin, 1980.
[16]. Rahnema F., Ravetto P., On the Equivalence on Boundary and boundary Condition Perturbations in Transport Theory*, Nuclear Sci. Eng.,* **128** (1998), 209-223.
[17]. Weston M., Stacey M., *Nuclear Reactor Physics,* Wiley, New York, 2001.