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APPLICATION OF RICHARDSON EXTRAPOLATION WITH THE CRANK–NICOLSON SCHEME FOR MULTI-DIMENSIONAL ADVECTION

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Abstract

Multi-dimensional advection terms are an important part of many large-scale mathematical models which arise in different fields of science and engineering. After applying some kind of splitting, these terms can be handled separately from the remaining part of the mathematical model under consideration. It is important to treat the multi-dimensional advection in a sufficiently accurate manner. It is shown in this paper that high order of accuracy can be achieved when the well-known Crank–Nicolson numerical scheme is combined with the Richardson extrapolation.

1. Multi-dimensional advection equations

Consider the multi-dimensional advection equation:

$$\frac{\partial c}{\partial t} = -\sum_{q=1}^{Q} u_q \frac{\partial c}{\partial x_q} \tag{1}$$

with $Q \geq 0$, $t \in [a,b]$ and $x_q \in [a_q, b_q]$ for $q = 1,2,\ldots,Q$. It is assumed that the coefficients $u_q = u_q(t, x_1, x_2, \ldots x_Q)$, $q = 1,2,\ldots,Q$, before the spatial partial derivatives in the right-hand-side of the partial differential equation (1) are some given functions.

Let D be the domain in which the independent variables involved in (1) vary and assume that:

$$(t, x_1, x_2, \dots x_Q) \in D \Rightarrow t \in [a, b] \ \wedge \ x_0 \in [a_q, b_q] \text{ for } q = 1, 2, \dots, Q. \qquad (2)$$

By applying the definition proposed in (2), it is assumed here that the obtained domain D is rather special (being a multi-dimensional parallelepiped), but this assumption is done only for the sake of simplicity. In fact, many of the results will also be valid for some considerably more complicated domains.

It will always be assumed that the unknown function $c = c(t, x_1, x_2, \dots, x_Q)$ is continuously differentiable up to some order $2p$ with $p \geq 1$ in all points of the domain D and with respect to all independent variables. Here p is the order of the numerical method which will be used in order to obtain some approximations of the unknown function at the points of some grid, which is appropriately selected (see below) in the domain defined in (2).

For some of the proofs, see [8], it will also be necessary to assume that continuous derivatives up to order two of all given functions u_q exist with respect of all independent variables.

The multi-dimensional advection equation (1) must always be considered together with some initial and boundary conditions.

The following notation in connection with some given positive increments h_q is useful in the proofs (see also [6]):

$$\overline{x} = (x_1, x_2, \dots, x_Q), \qquad (3)$$

$$\overline{x}^{(+q)} = (x_1, x_2, \dots, x_{q-1}, x_q + h_q, x_{q+1}, \dots, x_Q), \ q = 1, 2, \dots, Q, \qquad (4)$$

$$\overline{x}^{(-q)} = (x_1, x_2, \dots, x_{q-1}, x_q - h_q, x_{q+1}, \dots, x_Q), \ q = 1, 2, \dots, Q, \qquad (5)$$

$$\overline{x}^{(+0.5q)} = (x_1, x_2, \dots, x_{q-1}, x_q + 0.5h_q, x_{q+1}, \dots, x_Q), \ q = 1, 2, \dots, Q, \qquad (6)$$

$$\overline{x}^{(-0.5q)} = (x_1, x_2, \dots, x_{q-1}, x_q - 0.5h_q, x_{q+1}, \dots, x_Q), \ q = 1, 2, \dots, Q. \qquad (7)$$

2. Expanding the unknown function in Taylor series

The following result is very important in the efforts (see Section 6 and the conclusions in Section 7) to establish the order of accuracy which can be achieved when the Crank–Nicolson scheme is combined with the Richardson extrapolation.

Theorem 2.1 *Consider the multi-dimensional advection equation (1). Assume that* $(t, \overline{x}) \in D$ *is an arbitrary but fixed point and introduce the increments* $k > 0$ *and* $h_q > 0$ *such that* $t + k \in [a, b]$, $x_q - h_q \in [a_q, b_q]$ *and* $x_q + h_q \in [a_q, b_q]$ *for all* $q = 1, 2, \dots, Q$. *Assume furthermore that the unknown function* $c = c(t, \overline{x})$ *is continuously differentiable up to some order* $2p$ *with regard to all independent variables. Then there exists an expansion in Taylor series of the unknown function* $c = c(t, \overline{x})$ *around the point* $(t + 0.5k, \overline{x})$ *which contains terms involving only even degrees of the increments* k *and* h_q, $q = 1, 2, \dots, Q$.

Proof. The main ideas of the proof are quite straightforward (the unknown function c must be expanded in Taylor series and the series should be truncated after the first $2p$ terms), but it is rather long and complicated.
The full proof of Theorem 2.1 can be found in [8]. More precisely, the following equality is proved there:

$$\begin{aligned}\frac{c(t+k,\overline{x})-c(t,\overline{x})}{k} &= -\sum_{q=1}^{Q} u_q(t+0.5k,\overline{x})\frac{c(t+k,\overline{x}^{(+q)})-c(t+k,\overline{x}^{(-q)})}{4h_q} \\ &\quad -\sum_{q=1}^{Q} u_q(t+0.5k,\overline{x})\frac{c(t,\overline{x}^{(+q)})-c(t,\overline{x}^{(-q)})}{4h_q} \\ &\quad +\sum_{s=1}^{p} k^{2s}K^{(2s)} + \mathcal{O}(k^{2p+1}),\end{aligned} \tag{8}$$

where $K_t^{(2s)}$ and $K_q^{(2s)}$ are some constants and

$$K^{(2s)} = K_t^{(2s)} + \sum_{q=1}^{Q} \frac{h_q^{2s}}{k^{2s}} K_q^{(2s)}. \tag{9}$$

It should be noted here that it is assumed that all ratios h_q/k, $q=1,2,\dots,Q$, remain constants when $k \to 0$ (which can easily be achieved; for example by reducing all spatial increments h_q by a factor of two when the time-increment k is reduced by a factor of two).

3. Designing a second-order numerical method

Consider the grids:

$$G_t = \{t_n, n=0,1,\dots,N_t \mid t_0=a, t_n=t_{n-1}+k, n=1,2,\dots,N_t, k=\frac{b-a}{N_t}, t_{N_t}=b\} \tag{10}$$

and (for $q=1,2,\dots,Q$ and $h_q=(b_q-a_q)/N_q$)

$$G_x^{(q)} = \{x_q^{i_q}, i_q=0,1,\dots,N_q \mid x_q^0=a_q, x_q^{i_q}=x_q^{i_q-1}+h_q, i=1,2,\dots,N_q, x_q^{N_q}=b_q\}. \tag{11}$$

Introduce the following notations:

$$\tilde{x} = (x_1^{i_1}, x_2^{i_2}, \dots, x_Q^{i_Q}), \tag{12}$$

$$\tilde{x}^{(+q)} = (x_1^{i_1}, x_2^{i_2}, \dots, x_{q-1}^{i_{q-1}}, x_q^{i_q}+h_q, x_{q+1}^{i_{q+1}}, \dots, x_Q^{i_Q}), \tag{13}$$

$$\tilde{x}^{(-q)} = (x_1^{i_1}, x_2^{i_2}, \dots, x_{q-1}^{i_{q-1}}, x_q^{i_q}-h_q, x_{q+1}^{i_{q+1}}, \dots, x_Q^{i_Q}), \tag{14}$$

where $x_q^{i_q} \in G_x^{(q)}$ for $q=1,2,\dots,Q$.

In this notation the following numerical method can be defined:

$$\frac{\tilde{c}(t_{n+1},\tilde{x})-\tilde{c}(t_n,\tilde{x})}{k} \tag{15}$$
$$= -\sum_{q=1}^{Q} u_q(t_n+0.5k,\tilde{x})\frac{\tilde{c}(t_{n+1},\tilde{x}^{(+q)})-\tilde{c}(t_{n+1},\tilde{x}^{(-q)})+\tilde{c}(t_n,\tilde{x}^{(+q)})-\tilde{c}(t_n,\tilde{x}^{(-q)})}{4h_q}.$$

The computational device introduced by the finite difference equation (15) is often called the Crank–Nicolson scheme (see, for example, [5]). It is clear that (15) can be obtained from (8) by neglecting the terms in the last line and by assuming additionally that an arbitrary inner point of the grids defined by (10) and (11) is considered.

The quantities $\tilde{c}(t_n,\tilde{x})$ can be considered as approximations of the exact values of the unknown function $c(t_n,\tilde{x})$ at the grid-points from the grids defined by (10) and (11). It can easily be shown that the method introduced in (15) is of order two in respect to **all** independent variables.

Assume that the values of $\tilde{c}(t_n,\tilde{x})$ have been calculated for all grid-points of (11). Then the values $\tilde{c}(t_{n+1},\tilde{x})$ of the unknown function at the next time-point $t_{n+1} = t_n + k$ can be obtained by solving a huge system of linear algebraic equations of dimension $\tilde{N}$ where $\tilde{N}$ is defined by

$$\tilde{N} = \prod_{q=1}^{Q}(N_q-1). \tag{16}$$

4. Application of Richardson extrapolation

Consider (15) with $\tilde{c}$ replaced by z when $t = t_{n+1}$:

$$\frac{z(t_{n+1},\tilde{x})-\tilde{c}(t_n,\tilde{x})}{k} \tag{17}$$
$$= -\sum_{q=1}^{Q} u_q(t_n+0.5k,\tilde{x})\frac{z(t_{n+1},\tilde{x}^{(+q)})-z(t_{n+1},\tilde{x}^{(-q)})+\tilde{c}(t_n,\tilde{x}^{(+q)})-\tilde{c}(t_n,\tilde{x}^{(-q)})}{4h_q}.$$

Suppose that $0.5k$ and $0.5h_q$ are considered instead of k and h_q ($q = 1,2,\dots,Q$), respectively. Consider, as in formulae (5) and (6) but in the grid-points of the grids (10) and (11), the two vectors $\tilde{x}^{(+0.5q)} = (x_1^{i_1}, x_2^{i_2},\dots,x_{q-1}^{i_{q-1}}, x_q^{i_q}+0.5h_q, x_{q+1}^{i_{q+1}},\dots,x_q^{i_{N_q}})$ and $\tilde{x}^{(-0.5q)} = (x_1^{i_1}, x_2^{i_2},\dots,x_{q-1}^{i_{q-1}}, x_q^{i_q}-0.5h_q, x_{q+1}^{i_{q+1}},\dots,x_q^{i_{N_q}})$ for $q = 1,2,\dots,Q$.

Perform now additionally two small steps:

$$\frac{w(t_n+0.5k,\tilde{x})-\tilde{c}(t_n,\tilde{x})}{0.5k} \tag{18}$$
$$= -\sum_{q=1}^{Q} u_q(t_n+0.25k,\tilde{x})\frac{w(t_n+0.5k,\tilde{x}^{(+0.5q)})-w(t_n+0.5k,\tilde{x}^{(-0.5q)})}{4(0.5h_q)}$$
$$-\sum_{q=1}^{Q} u_q(t_n+0.25k,\tilde{x})\frac{\tilde{c}(t_n,\tilde{x}^{(+0.5q)})-\tilde{c}(t_n,\tilde{x}^{(-0.5q)})}{4(0.5h_q)}$$

$$\frac{w(t_n+k,\tilde{x})-w(t_n+0.5k,\tilde{x})}{0.5k} \tag{19}$$
$$= -\sum_{q=1}^{Q} u_q(t_n+0.75k,\tilde{x})\frac{w(t_n+k,\tilde{x}^{(+0.5q)})-w(t_n+k,\tilde{x}^{(-0.5q)})}{4(0.5h_q)}$$
$$-\sum_{q=1}^{Q} u_q(t_n+0.75k,\tilde{x})\frac{w(t_n+0.5k,\tilde{x}^{(+0.5q)})-w(t_n+0.5k,\tilde{x}^{(-0.5q)})}{4(0.5h_q)}.$$

The Richardson extrapolation can now be calculated by using the following formula (exploiting here the fact that the order of the underlying numerical method is of order of accuracy two in regard to all independent variables):

$$\tilde{c}(t_{n+1},\tilde{x}) = \frac{4w(t_{n+1},\tilde{x})-z(t_{n+1},\tilde{x})}{3}. \tag{20}$$

If the order of accuracy of the underlying method is not 2 but p, then the numbers 4 and 3 in (20) should be replaced by 2^p and 2^p-1, respectively.

5. Several general remarks on the Richardson extrapolation

Assume now that an arbitrary method of order p is used. Then, as mentioned above, (20) can be written as

$$\tilde{c}(t_{n+1},\tilde{x}) = \frac{2^p w(t_{n+1},\tilde{x})-z(t_{n+1},\tilde{x})}{2^p-1}. \tag{21}$$

The exact solution $c(t_{n+1},\tilde{x})$ can be expressed in the following two ways, where K is some constant and k is the time-increment:

$$c(t_{n+1},\tilde{x}) = z(t_{n+1},\tilde{x}) + k^p K + \mathcal{O}(k^{p+1}), \tag{22}$$
$$c(t_{n+1},\tilde{x}) = w(t_{n+1},\tilde{x}) + (0.5k)^p K + \mathcal{O}(k^{p+1}). \tag{23}$$

Eliminating the terms containing K in (22) and (23) gives:

$$c(t_{n+1},\tilde{x}) = \frac{2^p w(t_{n+1},\tilde{x})-z(t_{n+1},\tilde{x})}{2^p-1} + \mathcal{O}(k^{p+1}). \tag{24}$$

Denote:

$$\tilde{c}(t_{n+1}, \tilde{x}) = \frac{2^p w(t_{n+1}, \tilde{x}) - z(t_{n+1}, \tilde{x})}{2^p - 1}. \tag{25}$$

It is clear that the approximation $\tilde{c}(t_{n+1}, \tilde{x})$, being of order $p+1$, will be more accurate than both $z(t_{n+1}, \tilde{x})$ and $w(t_{n+1}, \tilde{x})$ when the stepsize k is sufficiently small. Thus, the Richardson extrapolation can be used in the efforts to improve the accuracy.

The Richardson extrapolation can also be used in an attempt to evaluate the leading term of the local error of the approximation $w(t_{n+1}, \tilde{x})$. Subtract (22) from (23), neglect the rest terms $\mathcal{O}(k^{p+1})$ and solve for K. The result is:

$$K = \frac{2^p[w(t_{n+1}, \tilde{x}) - z(t_{n+1}, \tilde{x})]}{k^p(2^p - 1)}. \tag{26}$$

Substitute K from (26) in (23):

$$c(t_{n+1}, \tilde{x}) - w(t_{n+1}, \tilde{x}) = \frac{w(t_{n+1}, \tilde{x}) - z(t_{n+1}, \tilde{x})}{2^p - 1} + \mathcal{O}(k^{p+1}), \tag{27}$$

which means that the quantity:

$$E_n = \frac{w(t_{n+1}, \tilde{x}) - z(t_{n+1}, \tilde{x})}{2^p - 1} \tag{28}$$

can be used as an evaluation of the local error of the approximation $w(t_{n+1}, \tilde{x})$ when the time-increment k is sufficiently small. If the evaluation of the local error computed by using (28) is not acceptable, then E_n can also be used to determine a new stepsize k which will hopefully give an acceptable error. Assume that the requirement for the accuracy imposed by the user is TOL. Then the new, hopefully better, time-increment k_{new} can be calculated by

$$k_{\text{new}} = \gamma \frac{TOL}{E_n} k, \tag{29}$$

where $\gamma < 1$ is used as a precaution factor, see for example [4]. Thus, the Richardson extrapolation can be applied in codes with automatic stepsize control.

The use of the Richardson extrapolation for stepsize control is relatively easy when systems of ordinary differential equations are solved numerically. The procedure becomes difficult when systems of partial differential equations are to be handled, because of the introduction of the assumption made in (9). This assumption implies that if k is multiplied by the factor $\gamma TOL/E_n$, then all h_q must be multiplied by the same factor in order to keep the ratios h_q/k constant. This difficulty can be avoided in the special case where all $K_q^{(2s)}$ are much smaller than $K_t^{(2s)}$. Then the Richardson extrapolation can be slightly modified so that all h_q are kept constant and only the time-stepsize k is to be controlled (thus, the situation becomes in principle the same as that appearing when systems of ordinary differential equations are treated).

It must be emphasized here that the Richardson extrapolation does not depend too much on the particular method used. It can be utilized both when classical numerical algorithms are applied in the solution of differential equations and when more advanced numerical methods which are combination of splitting procedures and classical numerical algorithms are devised and used. Two issues are important: (a) the large time-increment and the two small time-increments must be handled by the same numerical method and (b) the order p of the selected method should be known. If the Richardson extrapolation is used in connection with the multi-dimensional equation (1), then it is appropriate, see (9), to assume that for all values of q the ratios h_q/k are constants.

Much more useful details about different application issues related to the introduction of the Richardson extrapolation and its stability properties can be found in [2, 3, 9, 7, 10].

The above analysis shows that the accuracy order is as a rule increased by one. In the next section it will be shown that the application of the Richardson extrapolation in connection with the numerical method derived in Section 3 gives better accuracy when applied in the solution of (1).

6. Accuracy of Richardson extrapolation

Theorem 6.1 *Consider the multi-dimensional advection equation* (1). *Assume that the coefficients u_q before the spatial derivatives in* (1) *are continuously differentiable with respect to all independent variables and continuous derivatives of the unknown function c up to order four exist, again with respect to all variables. Then the combination of the numerical method* (15) *and the Richardson extrapolation is of order of accuracy four.*

Proof. The ideas, on which the proof is to be based, are quite clear. One must apply the result proved in Theorem 2.1 for $p = 2$ under an assumption that the numerical method defined by (15) is used at the grid-points of (10) and (11). However, the actual poof is very long and rather complicated. It can be found in [8]. It should be noted (see also Section 5) that in general the use of the Richardson extrapolation is leading to an increase of the accuracy order of the underlying numerical method by one. For the second-order numerical method (15) the accuracy order is increased by **two** (from order two to order four) when it is applied to the multi-dimensional advection equation (1) together with the Richardson extrapolation.

7. Conclusions

The result proved in this paper is a generalization of the result proved in [6], where the much simpler one-dimensional advection is handled.

It will be interesting to investigate whether the result proved in Theorem 6.1 for equation (1) can be extended for the more general multi-dimensional advection equation:

$$\frac{\partial c}{\partial t} = -\sum_{q=1}^{Q} \frac{\partial (u_q c)}{\partial x_q}, \; x_q \in [a_q, b_q] \text{ for } q = 1, 2, \ldots, Q \text{ with } Q \geq 1, \; t \in [a, b]. \qquad (30)$$

Richardson extrapolation can be repeatedly applied (see, for example, [1]). Theorem 6.1 indicates that when this is done, the order of accuracy will be increased by two after each successive application of the Richardson extrapolation. This remark explains why Theorem 2.1 is proved for an arbitrary value of p and not only for $p = 2$ as required in Theorem 6.1.

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