Richardson Extrapolated Numerical Methods for Treatment of One-Dimensional Advection Equations

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Abstract. Advection equations are an essential part of many mathematical models arising in different fields of science and engineering. It is important to treat such equations with efficient numerical schemes. The well-known Crank-Nicolson scheme will be applied. It will be shown that the accuracy of the calculated results can be improved when the Crank-Nicolson scheme is combined with the Richardson Extrapolation.
Key words: Advection equations, Numerical methods, Crank-Nicolson scheme, Richardson Extrapolation.

1 One-dimensional advection equations

Consider the advection equation:

$$(1) \qquad \frac{\partial c}{\partial t} = -u \frac{\partial c}{\partial x}, \qquad x \in [a_1, b_1] \subset (-\infty, \infty), \qquad t \in [a, b] \subset (-\infty, \infty).$$

The wind velocity $u = u(x, t)$ is some given function. Equation (1) must always be considered together with appropriate initial and boundary conditions. The well-known Crank-Nicolson scheme (see, for example, [2, p. 63]) can be applied in the numerical treatment of (1). The computations are carried out by the following formula:

$$(2) \qquad \begin{aligned} &\sigma_{i,n+0.5}\, c_{i+1,n+1} + c_{i,n+1} - \sigma_{i,n+0.5}\, c_{i-1,n+1} + \\ &+\sigma_{i,n+0.5}\, c_{i+1,n} - c_{i,n} - \sigma_{i,n+0.5}\, c_{i-1,n} = 0 \end{aligned}$$

when the Crank-Nicolson scheme is used. The quantity $\sigma_{i,n+0.5}$ is defined by

$$(3) \qquad \sigma_{i,n} = \frac{k}{4\,h}\, u(x_i, t_{n\,+\,0.5})$$

where $t_{n+0.5} = t_n + 0.5\,k$ and the increments h and k of the spatial and time variables are introduced by using two equidistant grids:

$$(4)\quad G_x = \left\{ x_i, i = 0, \ldots, N_x | \, x_0 = a_1, \, x_i = x_{i-1} + h, \, i = 1, \ldots, N_x, \, h = \frac{b_1 - a_1}{N_x} \right\}$$

$$(5)\quad G_t = \left\{ t_n, n = 0, \ldots, N_t \, | \, t_0 = a, \, t_n = t_{n-1} + k, \, n = 1, \ldots, N_t, \, k = \frac{b - a}{N_t} \right\}$$

2 Application of the Richardson Extrapolation

Assume that a one-dimensional hyperbolic equation similar to (1) is treated by an arbitrary numerical method, which is of order $p \geq 1$ with regard to the two independent variables x and t. Let $\{ z_{i,n+1} \}_{i=0}^{N_x}$ be the set of approximations of the solution of (1) calculated for $t = t_{n+1} \in G_t$ at all grid-points x_i, $i = 0, \, 1, \, \ldots, \, N_x$, of G_x (4) by using the numerical method chosen and the corresponding approximations $\{ z_{i,n} \}_{i=0}^{N_x}$ calculated at the previous time-step, i.e. for $t = t_n \in G_t$. Introduce vectors $\bar{c} \, (t_{n+1})$, $\bar{z}_n$ and $\bar{z}_{n+1}$ the components of which are $\{ c \, (x_i \, , \, t_{n+1}) \}_{i=0}^{N_x}$, $\{ z_{i,n} \}_{i=0}^{N_x}$ and $\{ z_{i,n+1} \}_{i=0}^{N_x}$ respectively. Since the order of the numerical method is assumed to be p with regard both to x and to t, we can write:

$$(6)\qquad \bar{c} \, (t_{n+1}) = \bar{z}_{n+1} + h^p K_1 + k^p K_2 + O \left(k^{p+1} \right) ,$$

where K_1 and K_2 are some quantities, which do not depend on h and on k. It is convenient to rewrite the last equality in the following equivalent form:

$$(7)\qquad \bar{c} \, (t_{n+1}) = \bar{z}_{n+1} + k^p K + O \left(k^{p+1} \right) , \qquad K \stackrel{def}{=} \left(\frac{h}{k} \right)^p K_1 + K_2 \, .$$

If h and k are sufficiently small, then the sum $h^p K_1 + k^p K_2$ will be a good approximation of the error in the calculated values of the numerical solution $\bar{z}_{n+1}$. If K is bounded, $| \, K \, | < \infty$, then $k^p K$ will also be a good approximation of the error of $\bar{z}_{n+1}$. This means that if we succeed to eliminate the term $k^p K$ in (7), then we shall obtain approximations of order $p + 1$. The Richardson Extrapolation can be applied in an attempt to achieve such an improvement of the accuracy. In order to apply the Richardson Extrapolation when (1) is treated by the Crank-Nicolson scheme it is necessary to introduce an additional grid:

$$(9)\qquad \begin{aligned} G_x^2 = \{ x_i \, , \; i = 0, \, 1, \, \ldots \, , \, 2N_x \, | \, x_0 = a_1 \, , \\ x_i = x_{i-1} + \tfrac{h}{2} \, , \; i = 1, \ldots, 2N_x \, , \; h = \tfrac{b_1 - a_1}{N_x} \right\} \, . \end{aligned}$$

Assume that approximations $\{ w_{i,n} \}_{i=0}^{2N_x}$ (calculated at the grid-points of G_x^2 for $t = t_n \in G_t$) are available and perform two small steps with a stepsize $k \, / \, 2$ to compute $\{ w_{i,n+1} \}_{i=0}^{2N_x}$. Use only the components with even indices i, $i = 0, \, 2, \, 4 \, , \, \ldots \, , \, 2N_x$ to form vector $\tilde{w}_{n+1}$. The following equality holds for this vector when the quantity K is defined as in (7):

$$(10) \qquad \bar{c}\,(t_{n+1}) = \tilde{w}_{n+1} + \left(\frac{k}{2}\right)^{p} K + O\left(k^{p+1}\right) \ .$$

It is possible to eliminate the quantity K from (7) and (10) by applying the following linear combination: multiply (10) by 2^p and subtract (7) from the result. Thus we obtain:

$$(11) \qquad \bar{c}\,(t_{n+1}) = \bar{c}_{n+1} + O\left(k^{p+1}\right) \ , \qquad \bar{c}_{n+1} \stackrel{def}{=} \frac{2^p\,\tilde{w}_{n+1} - \bar{z}_{n+1}}{2^p - 1} \, .$$

The approximation $\bar{c}_{n+1}$, being of order $p+1$, will be more accurate than both $\bar{z}_{n+1}$ and $\tilde{w}_{n+1}$ when h and k are sufficiently small. The device used to construct $\bar{c}_{n+1}$ is called Richardson Extrapolation (introduced in [1]). If the partial derivatives up to order $p+1$ exist and are continuous, then one should expect (11) to produce more accurate results than those obtained by the underlying numerical method.

Remark 1: The rest terms in the formulae given in this section will in general depend on both h and k. However, it is clear that h can be expressed as a function of k by using (7) and (6) and this justifies the use only of k in all rest terms.

Remark 2: No specific assumptions were made in this section, neither about the particular partial differential equation, nor about the numerical method used to solve it. This was done in order to demonstrate that the idea on which the Richardson Extrapolation is based is very general. However, it must be emphasized that in the remaining part of this paper it will always be assumed that (i) equation (1) is solved under the assumptions made in Section 1 and (ii) the underlying numerical algorithm used to handle it numerically is the second-order Crank-Nicolson scheme.

One should expect the combination of the Richardson Extrapolation and the Crank-Nicolson scheme to be a third-order numerical method. However, the actual result is much better, because the following theorem holds:

Theorem 1: *If $c(x,t)$ from (1) is continuously differentiable up to order five in both x and t, then the numerical method based on the Richardson Extrapolation and the Crank-Nicolson scheme is of order four.*

The Richardson Extrapolation can be implemented in four different manners depending on the way in which the computations at the next time-step, step $n+2$, will be carried out.

1. **Active Richardson Extrapolation:** Use $\bar{c}_{n+1}$ as initial value to compute $\bar{z}_{n+2}$. Use the set of values $\left\{ w_{i,n+1} \right\}_{i=0}^{2N_x}$ as initial values to compute $\left\{w_{i,n+2}\right\}_{i=0}^{2N_x}$ and $\tilde{w}_{n+2}$.

2. **Passive Richardson Extrapolation:** Use $\bar{z}_{n+1}$ as initial value to compute $\bar{z}_{n+2}$. Use the set of values $\{ w_{i,n+1} \}_{i=0}^{2N_x}$ as initial values to compute $\{ w_{i,n+2} \}_{i=0}^{2N_x}$ and $\tilde{w}_{n+2}$.
3. **Active Richardson Extrapolation with linear interpolation on the finer spatial grid (9):** Use $\bar{c}_{n+1}$ as initial values to compute $\bar{z}_{n+2}$. Set $w_{2i,n+1} = c_{i,n+1}$ for $i = 0, 1, \ldots, N_x$. Use linear interpolation to obtain approximations of the values of $w_{i,n+1}$ for $i = 1, 3, \ldots, 2N_x - 1$.Use the updated set of values $\{ w_{i,n+1} \}_{i=0}^{2N_x}$ as initial values to compute $\{ w_{i,n+2} \}_{i=0}^{2N_x}$ and $\tilde{w}_{n+2}$.
4. **Active Richardson Extrapolation with third-order interpolation on the finer spatial grid (9):** Use $\bar{c}_{n+1}$ as initial value to compute $\bar{z}_{n+2}$. Set $w_{2i,n+1} = c_{i,n+1}$ for $i = 0, 1, \ldots, N_x$. Use third-order Lagrangian interpolation polynomials to obtain approximations of $w_{i,n+1}$ for $i = 3, 5, \ldots, 2N_x - 3$ and second-order Lagrangian polynomials to obtain approximations of $w_{i,n+1}$ for $i = 1$ and $i = 2N_x - 1$ (i.e. to calculate $w_{1,n+1}$ and $w_{2N_x-1,n+1}$). Use the updated set of values $\{ w_{i,n+1} \}_{i=0}^{2N_x}$ as initial values to compute $\{ w_{i,n+2} \}_{i=0}^{2N_x}$ and $\tilde{w}_{n+2}$.

The improvements obtained by applying (11) are not used in the further computations when the Passive Richardson Extrapolation is selected. These improvements are partly used in the calculations related to the large step (only to compute $\bar{z}_{n+2}$) when the Active Richardson Extrapolation is used. An attempt to exploit the more accurate values also in the calculation of $\bar{w}_{n+2} = \{ w_{i,n+1} \}_{i=0}^{2N_x}$ is made in the last two implementations.

Information about the actual application of the third-order Lagrangian interpolation is given below. Assume that $w_{2i,n+1} = c_{i,n+1}$ for $i = 0, 1, \ldots, N_x$, i.e. the improved (by the Richardson Extrapolation) solution on the coarser grid (4) is projected at the grid-points with even indices $0, 2, \ldots, 2N_x$ of the finer grid (9). The interpolation rule used to get better approximations at the grid-points of (9) which have odd indices can be described by the following formula:

$$w_{i,n+1} = -\frac{3}{48} w_{i-3,n+1} + \frac{9}{16} w_{i-1,n+1} + \frac{9}{16} w_{i+1,n+1} - \frac{3}{48} w_{i+3,n+1}, \quad i = 3, 5, \ldots, 2N_x - 3. \tag{12}$$

Formula (12) is obtained by using a third-order Lagrangian interpolation for the case where the grid-points are equidistant and when an approximation at the mid-point x_i of the interval $[x_{i-3}, x_{i+3}]$ is to be found. Only improved values are involved in the right-hand-side of (12).
Formula (12) cannot be used to improve the values at the points x_1 and x_{N_x-1}. It is necessary to use second-order interpolation at these two points:

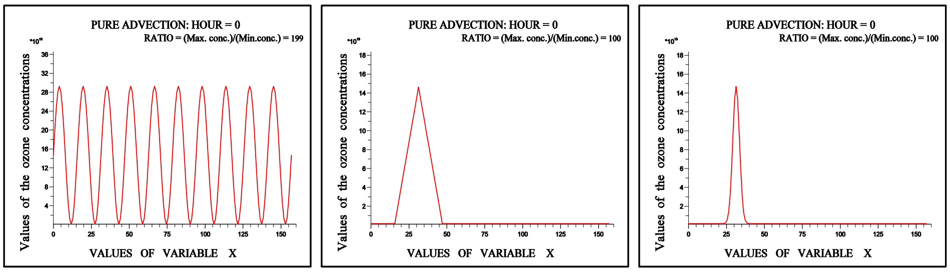
$$\begin{aligned} w_{1,n+1} &= \frac{3}{8} w_{0,n+1} + \frac{3}{4} w_{2,n+1} - \frac{1}{8} w_{4,n+1}, \\ w_{N_x-1,n+1} &= \frac{3}{8} w_{N_x,n+1} + \frac{3}{4} w_{N_x-2,n+1} - \frac{1}{8} w_{N_x-4,n+1}. \end{aligned} \tag{13}$$

3 Introduction of three numerical examples

An oscillatory example (EXAMPLE 1). Assume that the following relationships hold:

$$(14) \qquad \begin{array}{l} a = a_1 = 0\,, \qquad b = b_1 = 2\pi\,, \qquad u(x,t) = 0.5\,, \\ f(x) = [100 + 99\,\sin(10\,x)]\, *\, 1.4679 * 10^{12}\,. \end{array}$$

The exact solution of the problem defined by (14) is $c(x,t) = f(x - ut)$. Function $f(x)$ can be seen in Figure 1 a.



a) EXAMPLE 1 **b)** EXAMPLE 2 **c)** EXAMPLE 3

Fig. 1. The initial value conditions in the three examples. It is assumed that (i) there are 161 grid-points in the spatial interval and (ii) the initial values are ozone concentrations.

A discontinuous example (EXAMPLE 2). Another example is defined by the following relationships:

$$(15) \qquad x \in [0\,,\; 50\,000\,000]\;, \qquad t \in [43\,200\,,\; 129\,600]\;, \qquad u(x,t) = 320\; cm/s.$$

The distance is measured in centimetres, which means that the length of the spatial interval is 500 kilometres. The time is measured in seconds (starting in the mid-night). This means that the calculations are started at 12 o'clock and finished at the same time in the next day. The initial values are given by

$$(16) \qquad f(x) = 1.4679 * 10^{12} \quad \text{for} \quad x \le 5000000 \quad \text{or} \quad x \ge 15000000\;,$$

$$(17) \quad f(x) = \left[1 + 99 * \frac{x - 5000000}{5000000}\right] * 1.4679 * 10^{12}\,, \quad 5000000 \le x \le 10000000\,,$$

$$(18) \quad f(x) = \left[1 + 99 * \frac{15000000 - x}{5000000}\right] * 1.4679 * 10^{12}\,, \quad 10000000 \le x \le 15000000\,.$$

The exact solution of the problem defined by (15) – (18) is given by $c(x,t) = f(x - u(t - 43200))$. The variation of function $f(x)$ defined by (16) – (18) can be seen in Figure 1 b.

A smooth example with a sharp gradient (EXAMPLE 3). Assume that (15) holds and introduce:

$$(19) \qquad f(x) = \left(1 + e^{-\omega(x - 10\,000\,000)^2}\right) * 1.4679 * 10^{12}\,, \qquad \omega = 10^{-12}\,.$$

The exact solution of the problem defined by (15) and (19) is given by $c(x,t) = f(x - u(t - 43200))$. Function $f(x)$ from (19) can be seen in Figure 1 c. Similar example was used in [4].

Similar advection module is a part of the large-scale air pollution model UNI-DEM [3,5] and the quantities used in this section are either the same or very similar to the corresponding quantities in this model.

4 Numerical results

In each experiment the first run is performed by using $N_t = 168$ and $N_x = 160$. Ten additional runs are performed after the first one. When a run is finished, both h and k are halved (this means that N_t and N_x are doubled) and a new run is started. Thus, in the eleventh run we have $N_t = 172032$ and $N_x = 163840$. Note too, that the ratio h/k is kept constant and, therefore K from (7) remains bounded as required in (9).

We are mainly interested in the behavior of the numerical error. The error is evaluated at the end of every hour (i.e. 24 times in each run) at the grid-points of the coarsest spatial grid in the following way. Assume that run number $r\,,\quad r = 1\,,\ 2\,,\ \ldots\,,\ 11\,$, is to be carried out and let $R = 2^{r-1}$. Then the error is calculated by

$$(20) \qquad \begin{aligned} &ERR_m = \max_{j=0,1,\ldots,160} \left(\frac{\left| c_{\tilde{i},\tilde{n}} - c^{exact}_{\tilde{i},\tilde{n}} \right|}{\max\left(\left| c^{exact}_{\tilde{i},\tilde{n}} \right|, 1.0\right)} \right)\,, \\ &m = 0\,,\ 1\,,\ \ldots\,,\ 24\,, \qquad \tilde{i} = j\,R\,, \qquad \tilde{n} = 7\,m\,R\,, \end{aligned}$$

where $c_{\tilde{i},\tilde{n}}$ and $c^{exact}_{\tilde{i},\tilde{n}}$ are the calculated value and the reference solution at the end of hour m and at the grid-points of coarsest grid.
The global error made during the computations is estimated by using the following formula:

$$(21) \qquad ERR = \max_{m=1,2,\ldots,24} (ERR_m)\,.$$

Numerical results obtained in the runs of the above three examples are given in Table 1 – Table 3.

No	NT	NX	C-N only	Richardson Extrapolation [error (conv. rate)]			
				Active	Passive	Lin. interp.	3^{rd} order interp.
1	168	160	7.85E-01	2.04E-01	2.79E-01	3.83E-01	1.56E-02
2	336	320	2.16E-01	4.95E-02	7.14E-02	1.19E-01	1.23E-03 (12.7)
3	672	640	5.32E-02	1.25E-02	1.76E-02	2.47E-02	1.07E-04 (11.4)
4	1344	1280	1.33E-02	3.15E-03	4.33E-03	6.25E-03	1.15E-05 (9.3)
5	2688	2560	3.32E-03	7.87E-04	1.07E-03	1.57E-03	1.19E-06 (9.6)
6	5376	5120	8.30E-04	1.97E-04	2.67E-04	3.92E-04	1.48E-07 (8.1)
7	10752	10240	2.08E-04	4.92E-05	6.66E-05	9.81E-05	1.62E-08 (9.1)
8	21504	20480	5.19E-05	1.23E-05	1.66E-05	2.45E-05	1.96E-09 (8.2)
9	43008	40960	1.30E-05	3.08E-06	4.15E-06	6.13E-06	2.39E-10 (8.2)
10	86016	81920	3.24E-06	7.96E-07	1.04E-06	1.53E-06	3.24E-11 (7.4)
11	172032	163840	8.10E-07	1.92E-07	2.60E-07	3.83E-07	1.27E-11 (2.7)

Table 1: Running the oscillatory advection example (EXAMPLE 1) by using the Crank-Nicolson Scheme directly and in combination with four versions of the Richardson Extrapolation. The convergence rate is given in brackets for the last method.

No	NT	NX	C-N only	Richardson Extrapolation [error (conv. rate)]			
				Active	Passive	Lin. interp.	3^{rd} order interp.
1	168	160	1.34E-01	7.67E-02	7.93E-02	1.17E-01	4.98E-02
2	336	320	7.69E-02	4.42E-02	4.57E-02	6.66E-02	2.76E-02 (1.80)
3	672	640	4.42E-02	2.55E-02	2.56E-02	3.99E-02	1.55E-02 (1.78)
4	1344	1280	2.55E-02	1.64E-02	1.57E-02	2.45E-02	8.57E-03 (1.81)
5	2688	2560	1.64E-02	1.06E-02	1.07E-02	1.51E-02	4.59E-03 (1.87)
6	5376	5120	1.06E-02	5.80E-03	5.89E-03	9.68E-03	2.32E-03 (1.98)
7	10752	10240	5.80E-03	3.40E-03	4.09E-03	5.51E-03	1.19E-03 (1.95)
8	21504	20480	3.40E-03	2.35E-03	2.48E-03	3.23E-03	6.58E-04 (1.81)
9	43008	40960	2.35E-03	1.33E-03	1.10E-03	2.26E-03	2.38E-04 (2.75)
10	86016	81920	1.33E-03	9.29E-04	9.45E-04	1.14E-03	1.50E-04 (1.59)
11	172032	163840	9.36E-04	4.08E-04	2.99E-04	8.88E-04	2.79E-05 (4.94)

Table 2: Running the example with discontinuous derivatives (EXAMPLE 2) by using the Crank-Nicolson Scheme directly and in combination with four versions of the Richardson Extrapolation. The convergence rate is given in brackets for the last method.

No	NT	NX	C-N only	Richardson Extrapolation [error (conv. rate)]			
				Active	Passive	Lin. interp.	3^{rd} order interp.
1	168	160	7.37E-01	3.99E-01	3.78E-01	6.41E-01	1.45E-01
2	336	320	4.00E-01	1.27E-01	1.00E-01	3.34E-01	1.74E-02 (8.4)
3	672	640	1.25E-01	3.08E-02	1.28E-02	1.09E-01	1.22E-03 (14.2)
4	1344	1280	3.08E-02	7.76E-03	9.07E-04	2.67E-02	1.73E-05 (15.8)
5	2688	2560	7.77E-03	1.95E-03	5.37E-05	6.84E-03	4.84E-06 (16.0)
6	5376	5120	1.95E-03	4.89E-04	3.30E-06	1.72E-03	3.03E-07 (16.0)
7	10752	10240	4.89E-04	1.22E-04	2.07E-07	4.30E-04	1.89E-08 (16.0)
8	21504	20480	1.22E-04	1.23E-05	1.29E-08	1.07E-04	1.18E-09 (16.0)
9	43008	40960	3.09E-05	7.65E-06	8.09E-10	2.69E-05	7.61E-11 (15.5)
10	86016	81920	7.65E-06	1.91E-07	5.06E-11	6.72E-06	9.85E-12 (7.7)
11	172032	163840	1.91E-06	4.78E-07		1.68E-07	4.97E-12 (2.0)

Table 3: Running the smooth advection example (EXAMPLE 3) by using the Crank-Nicolson Scheme directly and in combination with four versions of the Richardson Extrapolation. The convergence rate is given in brackets for the last method.

Conclusions drawn by studying the results presented in Table 1:

- The Crank-Nicolson Scheme leads to second-order of accuracy when it is applied directly. This should be expected.
- The first three implementations of the Richardson Extrapolation (Active Richardson Extrapolation, Passive Richardson Extrapolation and Richardson Extrapolation with linear interpolation of the values of $\left\{ w_{i,n+1} \right\}_{i=0}^{2N_x}$ on the grid-points of the finer spatial grid) lead also to second-order accuracy (instead of the fourth-order accuracy which should be expected). On the other hand, these three methods give more accurate results than those obtained by using directly the Crank-Nicolson Method.
- The combination of the Crank-Nicolson Scheme with the Richardson Extrapolation performs as a third-order numerical method when it is enhanced with third-order Lagrangian interpolation polynomials for improving the accuracy of the values of $\left\{ w_{i,n+1} \right\}_{i=0}^{2N_x}$ on the finer spatial grid. Theorem 1 tells us that the combined method should be of order four. The lower accuracy achieved here is probably due to the use of interpolation of lower degree in formula (13).

Conclusions drawn by studying the results presented in Table 2:

- All five numerical methods (the direct implementation of the Crank-Nicolson Scheme and the four implementations of the Richardson Extrapolation) lead

to first-order of accuracy. This probably should be expected (because of the presence of discontinuities).
- The four implementations of the Richardson Extrapolation give more accurate results than those obtained by using directly the Crank-Nicolson Scheme.
- The combination of the Crank-Nicolson Scheme with the Richardson Extrapolation performs best when it is enhanced with third-order Lagrangian interpolation polynomials for improving the accuracy of the values of $\left\{ w_{i,n+1} \right\}_{i=0}^{2N_x}$ on the finer spatial grid. However, the improvements achieved are very modest also in this case.

Conclusions drawn by studying the results presented in Table 3:

- The direct application of the Crank-Nicolson Scheme leads to quadratic convergence.
- The active Richardson Extrapolation and the Richardson Extrapolation based on the use of linear interpolation behave as second order methods, but give slightly better accuracy than that obtained when the Crank-Nicolson scheme is applied directly.
- The Passive Richardson Extrapolation behaves as method of order four for this example.
- The fourth implementation of the Richardson Extrapolation behaves as a numerical method of order four. This result is in agreement with the statement of Theorem 1. We should mention that the interpolation formula (13) for the spatial boundary grid-points gives very accurate approximations for this particular example.

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