Extrapolation Techniques for the Numerical Solution of P.D.E.'s

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In the recent literature there have appeared a paper by Liu (2) dealing with a new explicit finite-difference method for solving parabolic P.D.E.'s and a communication by Wilkes (4) pointing out the validity (in terms of accuracy) of the implicit Crank-Nicholson method. This matter of the use of different finite-difference approximations is of more than casual interest, since Hlavacek (1) has stated that the Liu procedure is one of the best for simulating packed-bed reactor systems.

In this communication, however, we wish to point out that extrapolation techniques can be conveniently used as an overlay on the primary algorithm to yield a faster and more accurate algorithm with essentially a minimum of additional programming effort. On this basis it becomes evident that the distinctions between the explicit and implicit methods are of minor consequence.

To illustrate the viable features of the extrapolation algorithm, we select the linear P.D.E. of Liu:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \tag{1}$$

with initial condition

$$u(x, 0) = 0, \qquad 0 \leq x < 1 \tag{2}$$

and boundary conditions of

$$u(1, t) = 1, \qquad t > 0 \tag{3}$$

$$\frac{\partial u}{\partial x} = 0, \qquad x = 0,\ t > 0 \tag{4}$$

For the numerical solution we also add either

$$u(1, 0) = 0 \qquad \text{(Scheme } A\text{-Liu)} \tag{5A}$$

or

$$u(1, 0) = 1, \qquad \text{(Scheme } B\text{-Wilkes)} \tag{5B}$$

The basic algorithms used to solve (1)-(5*A*) or (1)-(5*B*) are

- Crank-Nicholson, implicit [*CN*]
- Saul'yev, alternating, initially right to left, explicit [*SRL*]
- Saul'yev, alternating, initially left to right, explicit [*SLR*]
- Saul'yev, averaging, explicit [*SA*]
- Liu, alternating, initially right to left, explicit [*LRL*]
- Liu, alternating, initially left to right, explicit [*LLR*]
- Liu, averaging, explicit [*LA*]

The distinction between the Saul'yev and Liu explicit forms has to do with the number of mesh points used on a constant-time line, two for Saul'yev and three for Liu. The interested reader is referred to Figure 1 of Liu's paper for further details.

To implement the extrapolation algorithm one solves the problem using any of the above specific algorithms for two or more sets of grid spacings. Combining these results in an appropriate extrapolation formula the truncation error may be reduced (increase the accuracy) beyond that associated with any of the specific grid spacings. The explicit extrapolation formula itself is determined by the form of the truncation error and the number of extrapolations. The work of Romberg as detailed by Wilf (3) for integrals serves as an excellent illustration of the concept. A detailed analysis of the theoretical and computational aspects of extrapolation will appear in a later publication from this laboratory.

All results to be quoted were run under a WATFØR compiler operating on the IBM 360/91 at the Princeton University Computing Center. Double precision was used throughout. Execution times quoted in seconds are accurate to ±10%.

To compare with the results of Liu and Wilkes we shall show the error in the calculated answers at $t = 0.1$ and $t = 0.5$ for $x = 0.2$, 0.6, and 0.8. The basic time and space grid spacings of $\Delta t = 0.002$ and $\Delta x = 0.05$ yield a $\rho = \Delta t/\Delta x^2 = 0.8$, which is taken as standard. For extrapolation we shall also report on the use of $\Delta t = 0.032$, $\Delta x = 0.2$, and $\Delta t = 0.008$, $\Delta x = 0.1$ ($\rho = 0.8$) combined for one extrapolation and then $\Delta t = 0.002$, $\Delta x = 0.05$ for two extrapolations. In addition, the pair of $\Delta t = 0.05$, $\Delta x = 0.2$ and $\Delta t = 0.0125$, $\Delta x = 0.1$ ($\rho = 1.25$) will be used for a single extrapolation. Note that in extrapolation large grid spacings are used initially followed by succes-

TABLE 1. |ERROR| $\times 10^5$ AT VARIOUS x AND t. NO EXTRAPOLATION

$t = 0.1$, $\Delta x = 0.05$, $\Delta t = 0.002$, $\rho = 0.8$
All data for Scheme A.

Method	$x = 0.2$	$x = 0.6$	$x = 0.8$
CN	121.4	244.4	175.3
*CN**	121.4	244.3	172.3
SA	217.8	251.7	231.6
*SA**	215.3	252.1	228.8
LA	351.3	239.6	133.7
*LA**	352.5	239.7	130.7
LLR	302.1	193.4	117.8
*LLR**	301.7	193.3	114.8

$t = 0.5$, $\Delta x = 0.05$, $\Delta t = 0.002$, $\rho = 0.8$

Method	Scheme	$x = 0.2$	$x = 0.6$	$x = 0.8$	Computing time
CN	*A*	91.3	56.5	29.7	2.14
CN	*B*	4.1	2.6	1.4	2.14
SRL	*A*	32.3	15.2	2.3	0.99
SRL	*B*	32.3	15.2	2.3	1.00
SLR	*A*	209.7	132.0	69.7	0.99
SLR	*B*	174.7	110.3	58.3	1.00
SA	*A*	119.9	71.9	33.4	1.39
SA	*B*	85.9	50.9	22.4	1.39
LRL	*A*	89.8	55.4	30.2	1.22
LRL	*B*	120.7	74.7	38.2	1.24
LLR	*A*	54.8	36.4	22.6	1.22
LLR	*B*	32.8	17.7	5.9	1.21
LA	*A*	71.9	45.4	25.6	1.34
LA	*B*	86.4	52.5	25.9	1.84

* Calculated independently by Wyman (5).

TABLE 2. |ERROR| × 10^5 AT VARIOUS x. ONE EXTRAPOLATION

All calculations start with $\Delta x = 0.2$.
Error is recorded at $t = 0.512$ for $\rho = 0.8$.
Error is recorded at $t = 0.5$ for $\rho = 1.25$.

Method	Scheme	ρ	$x = 0.2$	$x = 0.6$	$x = 0.8$	Computing time
CN	*A*	0.80	5.3	3.2	1.7	0.50
CN	*B*	0.80	6.1	3.9	2.0	0.54
CN	*A*	1.25	17.1	10.4	5.2	0.39
CN	*B*	1.25	14.2	9.1	4.6	0.42
SRL	*B*	0.80	382.8	182.2	75.4	0.34
SRL	*B*	1.25	525.4	185.6	43.4	0.30
SA	*B*	0.80	74.4	64.0	42.5	0.42
SA	*B*	1.25	190.9	160.6	92.5	0.32
LRL	*B*	0.80	122.6	34.4	3.4	0.39
LA	*B*	0.80	66.1	37.6	6.7	0.50

sively smaller spacings.

As an introduction to the extrapolation results, we present in Table 1 data on the standard case (no extrapolation). These correspond to extensions of Tables 1 and 2 of Liu. Of primary interest here is that these calculations completely confirm Wilke's comments on the validity of the Crank-Nicholson algorithm and also suggest that the errors given by Liu for the Saul'yev method were inordinately large. The results shown with an asterisk were an independent set of calculations. It is difficult to specify that any of the methods, *CN*, *S*, or *L*, are significantly better (more accurate or faster) than the others.

The superiority of the extrapolated results is apparent from Tables 1 to 3, with Tables 2 and 3 presenting extrapolated data. Using the Crank-Nicholson results as an illustration, we see that with one extrapolation we can achieve the accuracy of the nonextrapolation case but with one-quarter of the computing time. Two extrapolations show that for roughly the same computing time results can be obtained which are a thousandfold more accurate. Obviously, either in terms of higher accuracy or decreased computer time, the extrapolation algorithm is significantly better than the nonextrapolated procedure.

TABLE 3. |ERROR| × 10^5 AT VARIOUS x. TWO EXTRAPOLATIONS

All calculations start with $\Delta x = 0.2$.
Error is recorded at $t = 0.512$ for $\rho = 0.8$.
Error is recorded at $t = 0.5$ for $\rho = 1.25$.

Method	Scheme	ρ	$x = 0.2$	$x = 0.6$	$x = 0.8$	Computing time
CN	*A*	0.80	0.0146	0.0068	0.0031	2.36
CN	*B*	0.80	0.008	0.0034	0.0014	2.48
CN	*A*	1.25	0.075	0.042	0.0107	1.57
CN	*B*	1.25	0.009	0.0003	0.0177	1.66
SRL	*B*	0.80	30.4	13.3	3.04	1.00
SA	*B*	0.80	2.88	3.97	6.19	1.39
LRL	*B*	0.80	17.2	9.2	6.4	1.21
LA	*B*	0.80	0.2	1.4	1.6	1.89

Furthermore, these results show that of the three basic algorithms the Crank-Nicholson method is best when used in an extrapolation format.

Once again we emphasize that these results are given to show briefly the power of extrapolating known algorithms. A forthcoming publication will deal more specifically with aspects of the types of P.D.E.'s, with the form of truncation errors, with stability and round-off errors, with different modes of implementation of extrapolation, and with nonlinear problems.

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A Test of the Inertial Theory for Plate Withdrawal

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Consider the viscous entrainment of thin films of wetting liquids on flat supports by continuous steady state withdrawal. One of many bath arrangements for such a free coating process is shown in Figure 1. In particular, consider the prediction of film thickness h_0 (in the constant thickness region above the meniscus) as a function of constant withdrawal speed U_w, together with the influence of fluid properties (μ, σ, ρ). This problem has several applications in coating, cleaning, and lubrication processes (6). The mass flow rate entrained w by a plate of width b is related to the film thickness h_0 by the Nusselt type of expression

$$w = \rho\, U_w b h_0 \left[1 - \frac{h_0^2 \rho g}{3\mu U_w} \right] \tag{1}$$

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One new method of discussing this problem is to consider simultaneously the effect of four forces, namely that of inertia, surface tension, viscosity, and gravitational field. The nondimensional groups describing these four forces have been given (7) as fluid property number $Fp \equiv \mu(g/\rho\sigma^3)^{1/4}$, nondimensional speed $Ca \equiv U_w(\mu/\sigma)$, and thickness $D \equiv h_0(\rho g/\sigma)^{1/2}$. Thus the desired expression showing how thickness increases with speed may be described as

$$h_0 \left(\frac{\rho g}{\sigma}\right)^{1/2} = \phi_1 \left[\frac{U_w \mu}{\sigma}, \mu \left(\frac{g}{\rho\sigma^3}\right)^{1/4} \right] \tag{2}$$

or

$$D = \phi_1(Ca, Fp) \tag{2a}$$

One equivalent form of Equation (2a) involves Reynolds