A Potted History of Numerical PDEs

Dave Sloan's 60th Birthday Meeting
Strathclyde

December 16, 1998

- Richardson (1910)
- Courant, Friedrichs & Lewy (1928)
- Crank & Nicolson (1947)
- Mitchell (1950)
- Southwell & Allen (1955)

- Young (1954)
- Argyris (1954–55), Turner, *Clough*, Martin & Topp (1956) ("*the name FEM was proposed by Clough (1962)*" (Ciarlet).
- Peaceman & Rachford (1955)
- Dahlquist (1956)
- Lax & Wendroff (1960)

Richardson

The approximate arithmetical solution by finite differences of physical problems involving differential equations with applications to the stress in a masonry dam, Phil. Trans. Roy. Soc. London, A210, 307–357, 1910.

> *"The object of this paper is to develop methods whereby the differential equations of physics may be applied more freely than hitherto in the approximate form of difference equations to problems concerning irregular bodies."*

> *"Both for engineering and for many of the less exact sciences, such as biology,there is a demand for rapid methods. . . "*

> *"The extension to three variables is, however, perfectly obvious. One has to let the third variable be represented by the number of pages of a book of tracing paper."*

> *"Having solved an equation . . . it remains to enquire how much in error the integral might be. A rule of apparent universal application is to take smaller co-ordinate differences and repeat the integration; and, if necessary, extrapolate in the manner explained below"* (Richardson Extrapolation, 1927)*.

**The deferred approach to the limit*, Phil. Trans. Roy. Soc. London, Ser. A, vol. 226,229–361, 1927

Notation

$\frac{\partial u}{\partial x}$ approximated by $\mu \frac{\eth u}{\eth x} = \frac{1}{2h}\{(10) - (\bar{1}0)\}$

$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$ approximated by $\frac{\eth^2 u}{\eth^2 x} + \frac{\eth^2 u}{\eth^2 y} = \triangleright^2 u$

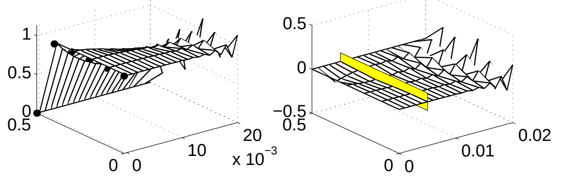
$$= \frac{1}{h^2}\left[(10) + (01) + (\bar{1}0) + (0\bar{1}) - 4(00)\right]$$

By the time of CFL (1928), the notation had changed to

$$\mu \frac{\eth u}{\eth x} = \frac{1}{2}[u_x + u_{\bar{x}}]$$
$$\triangleright^2 u = u_{x\bar{x}} + u_{y\bar{y}}$$

Richardson - The Heat Equation

"The method of this example is so simple that it can hardly be novel."



Richardson's computation for the heat equation on $-\frac{1}{2} < x < \frac{1}{2}$ carried on for 20 time steps:

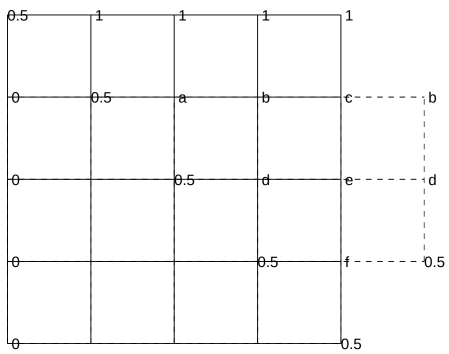
$$h = 1/10, \qquad \Delta t = 0.001$$

$$U_m^{n+1} = U_m^{n-1} + 2\frac{\Delta t}{h^2}\left(U_{m+1}^n - 2U_m^n + U_{m-1}^n\right)$$

Richardson and Laplace's equation

$$\triangleright^2 U = 0, \qquad \text{in} \quad (-1,1)\times(-1,1)$$

with $U = 0$ on two opposite edges & $U = 1$ on the other two edges.



"The solution of these six simultaneous equations was accomplished in an hour..."

$$\begin{bmatrix} 4 & -1 & 0 & 0 & 0 & 0 \\ -1 & 4 & -1 & -1 & 0 & 0 \\ 0 & -2 & 4 & 0 & -1 & 0 \\ 0 & -1 & 0 & 4 & -1 & 0 \\ 0 & 0 & -1 & -2 & 4 & -1 \\ 0 & 0 & 0 & 0 & -1 & 4 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \\ e \\ f \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \\ 1 \\ 1 \\ 0 \\ 3/2 \end{bmatrix}$$

$$u = \frac{4}{\pi}\sum_{m=1}^{\infty}(-1)^m \frac{\operatorname{sech}(2m-1)\frac{\pi}{2}}{2m-1}\cos(2m-1)x\cosh(2m-1)y.$$

"Adding up the series at these six points took 3 hours."

"So far I have paid piece rates for the operation $\eth_x^2 + \eth_y^2$ of about $\frac{n}{18}$ pence per coordinate point, n being the number of digits. The chief trouble to the computers has been the intermixture of plus and minus signs. As to the rate of working, one of the quickest boys averaged 2000 operations $\eth_x^2 + \eth_y^2$ per week, for three digits., those done wrong being discounted."

Richardson's Iterative Method

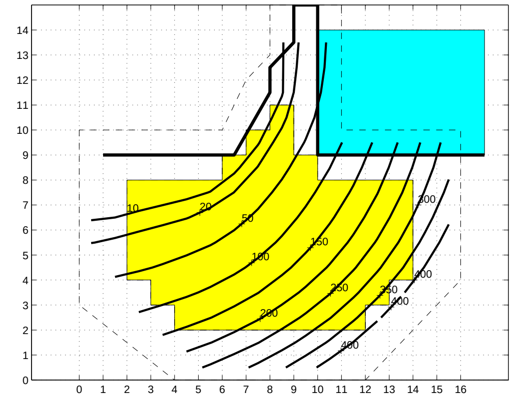
For the discrete Laplacian, this would be

$$U^{n+1} = U^n - \alpha_n \nabla^2 U^n$$

$n = 0, 1, \ldots$ and the sequence $\{\alpha_n\}$ are often chosen cyclically (See also Varga). Richardson was aware of the fact that the $\{\alpha_n\}$ should be chosen so that the "iteration polynomial" should be small on the spectrum of the iteration matrix.

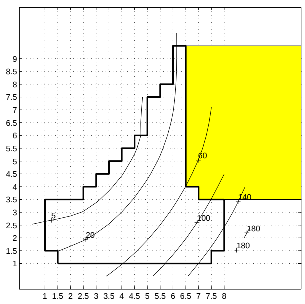
> *". . . can be done by clerks who need not understand algebra or calculus. Small and infrequent mistakes, or taking only a small number of digits, do not prevent one arriving at a fairly correct result. Nevertheless, it has been found best to have everything worked in duplicate."*

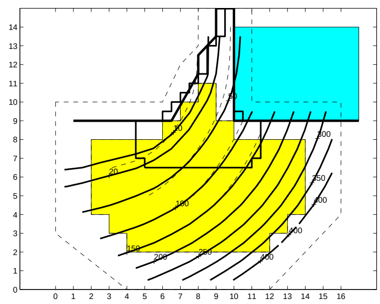
Richardson's Dam Problem



Contours of the stress function χ which satisfies

$$(\nabla^2)^2 \chi = 0$$





"The multiplications were made with a 20 inch slide rule"

Richardson & Weather

> *"During the battle of Champagne in April 1917 the working copy was sent to the rear, where it became lost, to be rediscovered some months later under a heap of coal"* *

> *". . . the preference for momentum-per unit volume rather than that of velocity. . ."* (Finite Volume Scheme)

> *". . . it would be necessary that the number of meridians be divisible by 2 many times over. For instance, instead of 120 meridians 3° apart, it would be better to have $2^7 = 128$ meridians. . . unfortunately this was not thought of until. . ."*

**Weather Prediction by Numerical Process*, 1922, Cambridge University Press.

"If the time step were 3 hours, then 32 individuals could just compute two points so as to keep pace with the weather... if the coordinate chequer were 200km square in plan... so that 64,000 computers would be needed to race the weather for the whole globe. That is a staggering figure. ... the organisation indicated is a central forecast factory..."

"Perhaps some day in the dim future it will be possible to advance the computations faster than the weather advances... But that is a dream."

Courant, Friedrichs & Lewy

Über die partiellen Differenzengleichungen der mathematischen Physik, Math. Ann., **100**,32–,1928*

Main Results: **Laplace's Equation**

Domain $\mathcal{G}$ is simply connected with boundary composed of finite number of arcs with continuous tangents. Grid $\mathcal{G}_h$ square of side h. *As $h \to 0$, $u_h(x,y)$ converges to a function $u(x,y)$ satisfying $\nabla^2 u = 0$ and takes the value $f(x,y)$ on the boundary. We shall show further that for any region lying entirely within $\mathcal{G}$ the difference quotients of u_h of arbitrary order tend uniformly towards the corresponding partial derivatives of $u(x,y)$.*

Methodology: Variational , based on discrete bilinear forms and penalty methods to satisfy the boundary conditions.

Generalisation: Biharmonic equation.

**On the partial differential equations of Mathematical Physics*, AEC Res. & Dev. Report, NYO-7689, New York University, 1956

CFL: The Wave Equation

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

approximated by $u_{t\bar{t}} = u_{x\bar{x}}$ with time steps Δt and space steps Δx.

Result *If $\Delta x < \Delta t$ and one lets $\Delta t \to 0$, then the solution of the difference equation* **cannot** *converge to the solution of the differential equation.*

Method of Proof depends on the now familiar ideas of domain of dependence and quadratic forms (L_2 theory).

Generalisation to two space dimensions: $2u_{t\bar{t}} = u_{x\bar{x}} + u_{y\bar{y}}$ and characteristic cones.

CFL & the Heat Equation

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

is approximated by

$$U_j^{n+1} = \tfrac{1}{2}[U_{j-1}^n + U_{j+1}^n]$$

i.e. with $\Delta t = \Delta x^2$ ($r = 1/2$ in standard notation). and $U_j^0 = f_{2j}$, $j = 0, \pm 1, \pm 2, \ldots$ (Pure IVP) Then

$$u(0,t) = \sum_{j=-n}^{n} \frac{1}{2^{2n}} \binom{2n}{n+j} f_{2j}$$

with $t = 2nh^2$. They show that this sum converges to

$$u(x,0) = \frac{1}{\sqrt{2\pi t}} \int_{-\infty}^{\infty} \mathrm{e}^{-\xi^2/2t} f(\xi) \mathrm{d}\xi.$$

J. Crank & P. Nicolson

A practical method for numerical evaluation of solutions of partial differential equations of the heat-conduction type, Proc. Camb. Phil. Soc., **43**, 50–67, 1947

Problem:

$$\frac{\partial\theta}{\partial t} = \frac{\partial^2\theta}{\partial x^2} - q\frac{\partial w}{\partial t}$$

$$\frac{\partial w}{\partial t} = -kw\mathrm{e}^{-\frac{A}{\theta}}$$

$$\theta_x|_{x=0} = H_1(\theta), \qquad \theta_x|_{x=1} = H_2(\theta).$$

$\theta(x, 0)$, $w(x, 0)$ both given.

Application: Burning of wood to form charcoal.

Method I

Discretisation in time to give a sequence of BVPs.

$$\begin{aligned}\frac{1}{\Delta t}[\theta^{n+1}(x) - \theta^n(x)] &= \frac{1}{2}\frac{\partial^2}{\partial x^2}[\theta^{n+1}(x) + \theta^n(x)] \\ &\quad - \frac{q}{\Delta t}[w^{n+1} - w^n]\end{aligned}$$

$$\begin{aligned}w^{n+1} &= w^n\mathrm{e}^{2E} \\ E &= -\tfrac{1}{2}k\Delta t\,\exp\left(-\frac{2A}{\theta^{n+1}(x) + \theta^n(x)}\right)\end{aligned}$$

The above equation for w^{n+1} being preferred (Hartree) to the "Trapezoidal" approximation with

$$\mathrm{e}^{2E} \Rightarrow \frac{1+E}{1-E}.$$

Method I—Solution

The basic idea was a shooting technique:

> "*. . . evaluating a number of solutions starting at $x = 0$, with different initial values for $\theta^{n+1}(0)$ and by trial and error finding a solution which satisfied the condition $\theta_x|_{x=1} = 0$. This may necessitate* **six or more trial solutions for each step** *in time. . . furthermore, three operators were required to feed the differential analyser the functions. . . only four integrator units of the analyser are needed. . .*"

Method II

Method of Lines - the spatial derivatives are replaced by differences and the differential analyser used to solve the resulting system of ODEs, a method much favoured by Hartree for the heat equation. . .

> . . . adequate accuracy was obtained by taking 3 or 4 intervals Δx (and) it was possible to use an 8-integrator differential analyser* to solve the resulting 4 or 5 ordinary equations.

The system looked at by Crank and Nicolson doubled the number of ODEs and overwhelmed the hardware.

* "the largest machine at present available in Great Britain"

Method III—The C-N Method

$$(1+r)\theta_m^{n+1} = \tfrac{1}{2}r\left[\theta_{m-1}^{n+1}+\theta_{m-1}^{n+1} + \theta_{m-1}^{n}+\theta_{m-1}^{n}\right] + (1-r)\theta_m^n - q[w^{n+1}-w^n],$$

$$w^{n+1}-w^n = w^n e^{2E_m^{n+1/2}}.$$

$$r = \frac{\Delta t}{\Delta x^2}.$$

Solution process:

“. . . at iterative method of solution, in some ways similar to the Southwell relaxation process. . . it is rarely necessary to iterate more than twice.”

Comparison of Methods

Method III ($w=0$—heat equation)

“. . . the computation of a single line with Δx= 1/8 takes under 10 min. which is considerably quicker than evaluation of the formal solution, for the same number of points.”

	Method		No. of operators required	Approximate time for 1 complete solution
I.	Finite steps in t Integrate in x	Differential Analyser	3	2 weeks
II.	3 steps in x Integrate in t	Differential Analyser	2	3-4 hours
III.	Finite steps in x and t C-N Method		1	7–8 hrs. ($\Delta x=\frac{1}{8}$) 10–12 hrs. ($\Delta x=\frac{1}{12}$)

Crank-Nicolson & von Neumann

“An alternative way of examining the accumulation of errors in the case of Richardson's process was proposed to the authors by Prof. D. R. Hartree, following a suggestion by Prof. J. von Neumann.”

“The error $\Delta\theta$ to which θ is subject must satisfy the same difference equation as does θ. . . and takes the form”

$$\Delta\theta_m^n = \sum_{j=1}^{P} f_j(n\Delta t)\sin[(2j-1)m\pi\Delta x/2]$$

“. . . the general solution (of Richardson's method) is

$$f_j(n\Delta t) = A_j e^{nk_1\Delta t} + B_j(-1)^n e^{-nk_1\Delta t}$$

from which they conclude that the method is unconditionally unstable.

The von Neumann Method for Stability Analysis

“The partly heuristic technique for stability analysis developed by von Neumann was applied by him to a wide variety of difference and differential equation problems during World War II. . . With the kind permission of Professor von Neumann, we have made (such) a discussion part of the present paper.” *

This paper contains the “von Neumann Method” as we know it: at a grid point (x,t), the error is expressed as

$$E(x,t) = e^{\alpha(\beta)t}e^{i\beta x}$$

and we write $\xi = e^{\alpha t}$.

*From: *A study of the numerical solution of partial differential equations*, G. G. O'Brien, M. A. Hyman & S. Kaplan. J. Math. Physics, **29**, 223–251 (1951).

A R Mitchell

Relaxation Methods in Compressible Flow, Pd D Thesis, St Andrews, (1950?)

$$\nabla^2(\chi\psi) - \psi\nabla^2\chi = 0$$

$$\frac{2}{\gamma-1}\left(1-\left(\frac{\chi}{\chi_0}\right)^{2(1-\gamma)}\right) = \frac{\chi^4}{c_0^2}\left(\left(\frac{\partial\chi}{\partial x}\right)^2 + \left(\frac{\partial\chi}{\partial y}\right)^2\right)$$

> *"Professor R V Southwell and Professor H W Emmons asserted that the relaxation technique fails to yield definite results under supersonic conditions, but this it is hoped to disprove in the course of the investigation."*

> *". . . compression shocks will always be discontinuities added to the flow obtained by the relaxation technique."*

Southwell & Allen

Relaxation methods applied to determine the motion in two dimensions of a viscous fluid past a fixed cylinder, Quart. J. Mech. Appl. Math., 129–145,**8**, 1955.*

Steady Navier-Stokes in transformed variables:

$$\alpha = x\left(1+\frac{1}{4(x^2+y^2)}\right), \quad \beta = y\left(1-\frac{1}{4(x^2+y^2)}\right)$$

$$\frac{\partial^2\psi}{\partial\alpha^2} + \frac{1}{R}\frac{\partial^2\psi}{\partial\beta^2} = -\frac{\zeta}{h^2}$$

$$\frac{\partial^2\zeta}{\partial\beta^2} + \frac{\partial\psi}{\partial\alpha}\frac{\partial\zeta}{\partial\beta} + \frac{1}{R}\left(\frac{\partial^2\zeta}{\partial\alpha^2} - R\frac{\partial\psi}{\partial\beta}\frac{\partial\zeta}{\partial\alpha}\right) = 0$$

Let $\kappa = \psi_\alpha$ and rewrite the 2nd equation as

$$\frac{\partial^2\zeta}{\partial\beta^2} + \kappa\frac{\partial\zeta}{\partial\beta} = A$$

which, assuming that κ, A are constant, gives

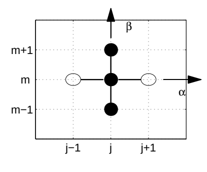
$$\kappa\zeta = A\beta + P + Qe^{-\kappa\beta}$$

**"This investigation, started in 1944, was frequently interrupted on account of pressure of more immediately urgent problems. An interim. . . 1948. . . . aided financially by the Worshipful company of Clothworkers."*

$$\kappa\zeta = A\beta + P + Qe^{-\kappa\beta}$$

Now choose P, Q so that

$$\zeta = \zeta_{j,m-1} \quad \text{at} \quad \alpha = j\Delta\alpha, \beta = (m-1)\Delta\beta$$
$$\zeta = \zeta_{j,m+1} \quad \text{at} \quad \alpha = j\Delta\alpha, \beta = (m+1)\Delta\beta$$



Then the method is defined by

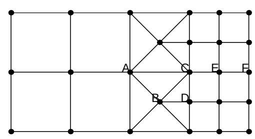
$$\kappa_{j,m}\zeta_{j,m} = [A\beta + P + Qe^{-\kappa\beta}]_{j,m}$$

This is the **Allen & Southwell scheme** (devised by Allen) and often attributed to Il'in*

Differencing scheme for a differential equation with a small parameter affecting the highest derivative*, Math. Notes Acad. Sci. USSR, **6, 592–602(1969)

Stencils & Relaxation

Relaxation Methods in Engineering and Science, D N de G Allen, McGraw Hill, 1954.



Allen & the Heat Equation

He begins with Richardson's Method for $u_t = u_{xx}$

$$U_m^{n+1} = U_m^{n-1} + 2\frac{\Delta t}{h^2}\left(U_{m+1}^n - 2U_m^n + U_{m-1}^n\right)$$

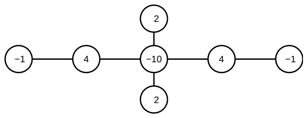
but abandons this because the equations cannot be solved by relaxation methods—he attributes this to the fact that it is first order in time. He proceeds to make a substitution

$$u = \frac{\partial v}{\partial t} + \kappa\frac{\partial^2 v}{\partial x^2}$$

leading to

$$v_{tt} = \kappa^2 v_{xxxx}$$

which is approximated by central differences (with $\Delta t = h^2/\kappa\sqrt{2}$)*



$$\begin{array}{lll} v_t + \kappa v_{xx} = 0 & \text{at} & t = 0 \\ v_t & \text{at} & t = T \\ v = v_{xx} = 0 & \text{at} & x = 0, 1 \end{array}$$

* *"It can be seen at once that (the full set of conditions) are of a kind whose satisfaction does not lead to any computational difficulty"*