A Brief History of Numerical Libraries

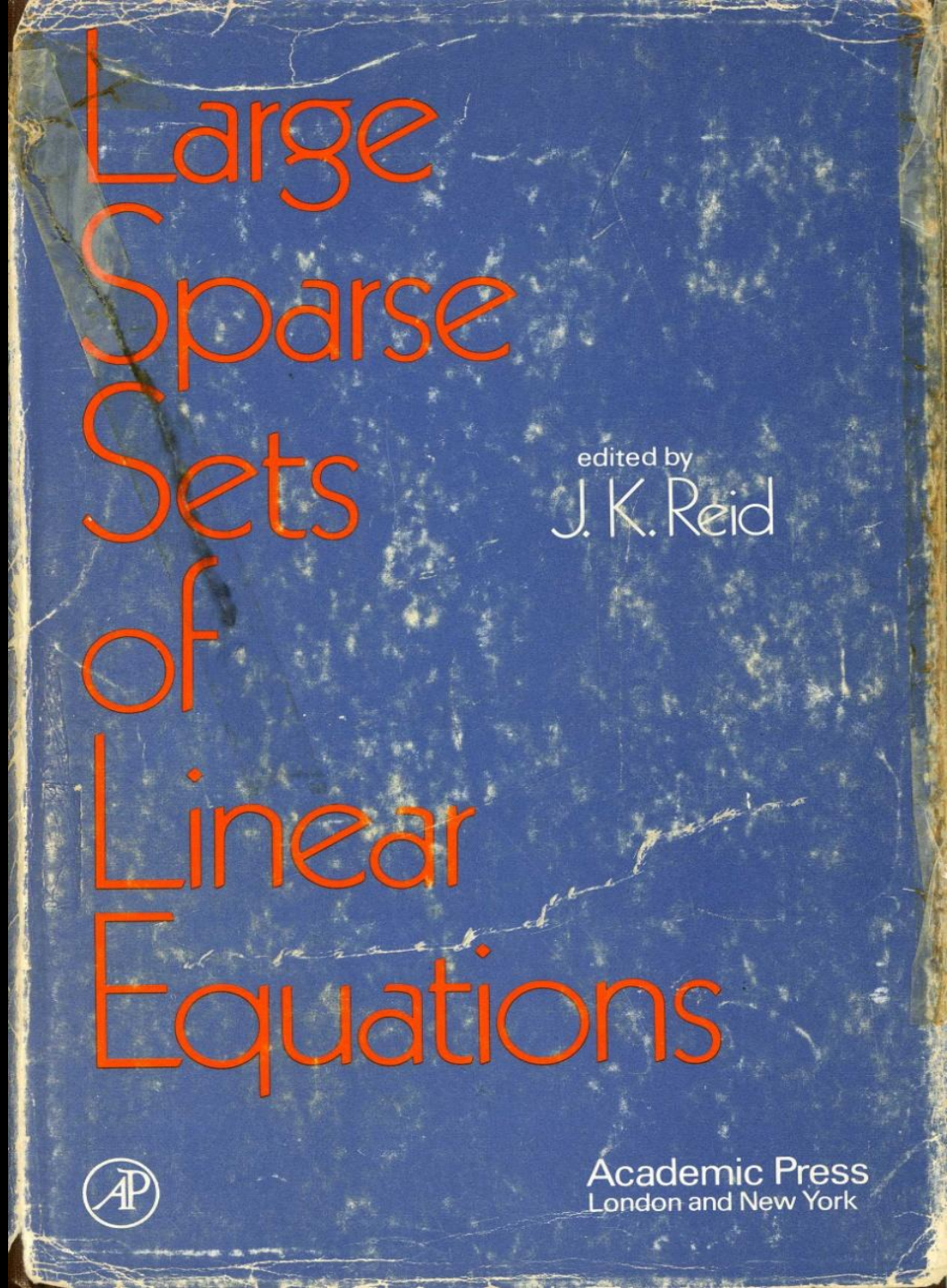
Sven Hammarling
NAG Ltd, Oxford
&
University of Manchester

John Reid at Gatlinburg VII (1977)

"Solution of large finite element systems of linear equations out of main storage"

Proceedings of IMA Conference, Oxford, 1970

Published 1971



John's Article on CG

On the Method of Conjugate Gradients for the Solution of Large Sparse Systems of Linear Equations

J. K. Reid

Mathematics Branch, Atomic Energy Research Establishment Harwell, England.

1. Introduction

The method of conjugate gradients has been known for some time, having been developed independently by E. Stiefel and by M. R. Hestenes with the co-operation of J. B. Rosser, G. Forsythe and L. Paige, but it has received little attention recently. It is difficult to see why this has been so since the method has several very pleasant features when regarded not as a direct method for the solution of full systems of equations but as an iterative method for the solution of large and sparse systems. It is our purpose here to explain these features and to report on some numerical experiments which compare the various versions of the algorithm that are available.

2. The Algorithm and its Variants

We will follow the notation of Hestenes and Stiefel [1] because their original algorithm has advantages over other versions of the method that have been proposed subsequently. Given a system

$$Ax = b \tag{2.1}$$

of n linear equations whose matrix A is symmetric and positive-definite we take a starting vector x_0, form the corresponding residual

$$r_0 = b - Ax_0, \tag{2.2}$$

set $p_0 = r_0$ and then for $i = 0, 1, 2, \ldots$ find the vectors x_{i+1}, r_{i+1} and p_{i+1} and the scalars a_i and b_i by using the recursions

$$a_i = \begin{cases} \text{either } (p_i, r_i)/(p_i, Ap_i) & \text{(2.3a)} \\ \text{or } \quad (r_i, r_i)/(p_i, Ap_i) & \text{(2.3b)} \end{cases}$$

John's CG Article

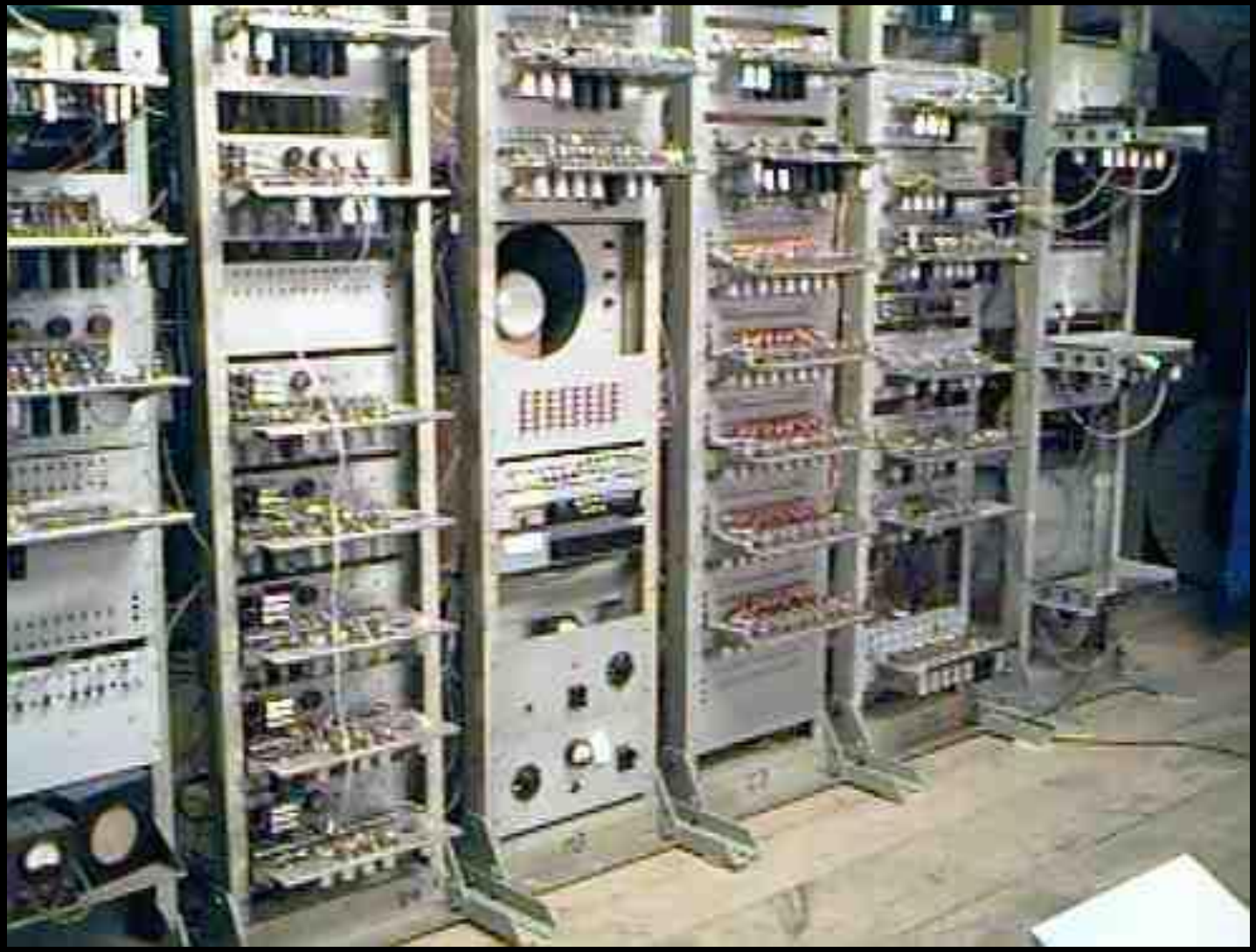
"The paper of Reid (1971) drew the attention of many researchers to the potential of the algorithm as an iterative method for sparse linear systems. It was a catalyst for much of the subsequent work in conjugate gradients."

Golub and O'Leary, SIAM Review, 1989

Rough Outline

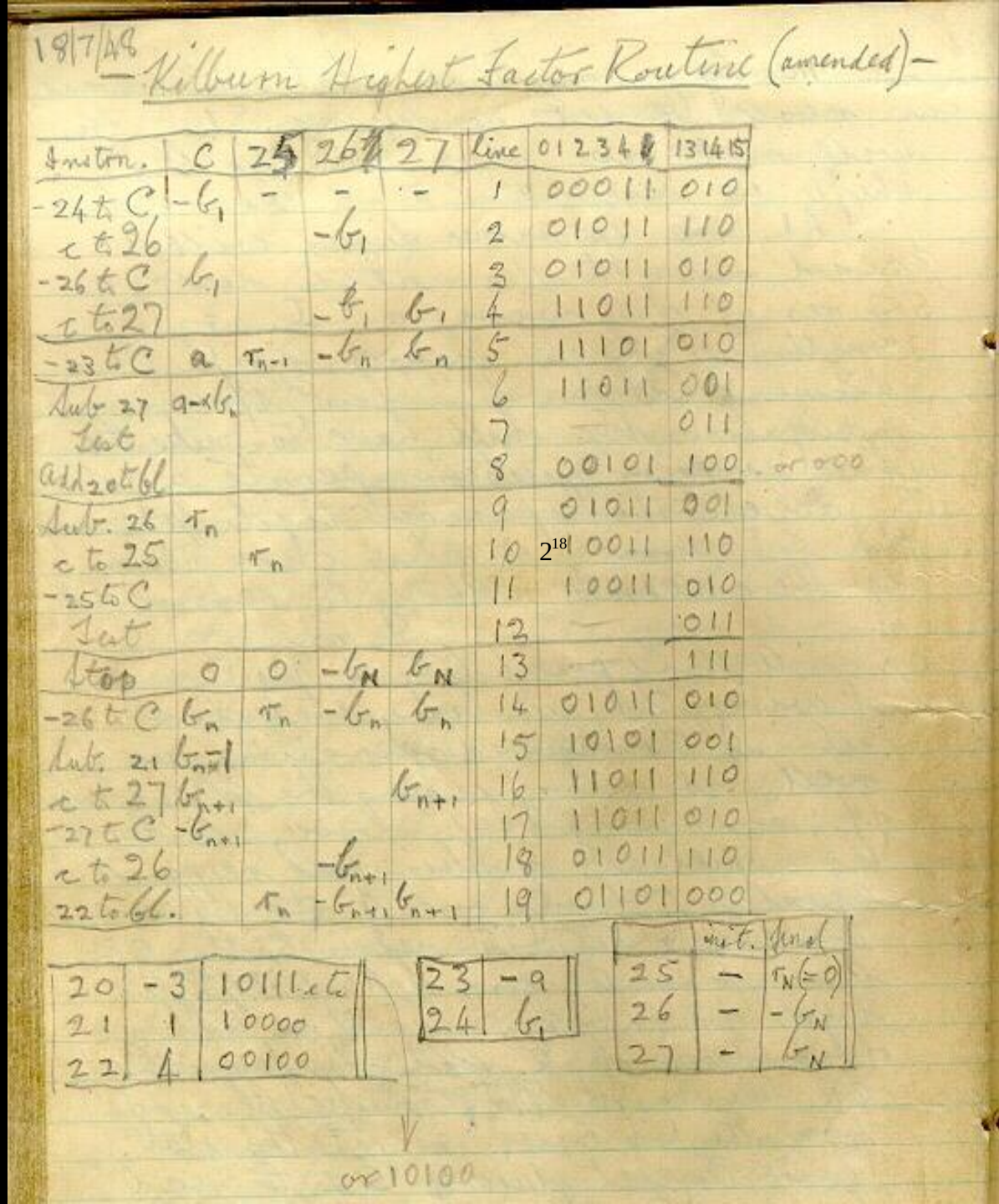
- History
- Libraries, packages and their facets
- Fortran
- Floating Point Arithmetic
- Proceedings and Books
- Summary

Manchester Baby, 21 June 1948 (Replica)



Kilburn/Tootill Program to compute the highest proper factor

2^{18} took 52 minutes
1.5 million instructions
3.5 million store accesses



First Numerical Library

Wilkes, Wheeler and Gill (1951) “Preparation of Programmes for an Electronic Digital Computer” Addison-Wesley

With special reference to the EDSAC and the use of a library of subroutines

“Short, ready-made programs for performing the more common computing operations … are usually called subroutines” (page 1)

Wilkes, Wheeler and Gill

For V:

$z \leftarrow x \pm y$

$y \leftarrow Ax, \quad A = A^T$

PART II

SPECIFICATIONS OF LIBRARY SUBROUTINES

Each subroutine is distinguished by a letter denoting its category and a serial number within that category. The categories are as follows.

Category	Subject
A	Floating point arithmetic.
B	Arithmetical operations on complex numbers.
C	Checking.
D	Division.
E	Exponentials.
F	General routines relating to functions.
G	Differential equations.
J	Special functions.
K	Power series.
L	Logarithms.
M	Miscellaneous.
P	Print and layout.
Q	Quadrature.
R	Read (i.e., Input).
S	nth root.
T	Trigonometrical functions.
U	Counting operations.
V	Vectors and matrices.

In the specifications on succeeding pages the following information is given in abbreviated form immediately beneath the title of each subroutine:

1. Type of subroutine, i.e., whether open, closed, interpretive, or special.
2. Restriction on address of first order. If the word "even" appears it denotes that the first order must have an even address; if no note appears it indicates that the address may be either odd or even.
3. Total number of storage locations occupied by the subroutine.
4. Addresses of any storage locations needed as working space by the subroutine.
5. Approximate operating time (not possible to state in all cases).

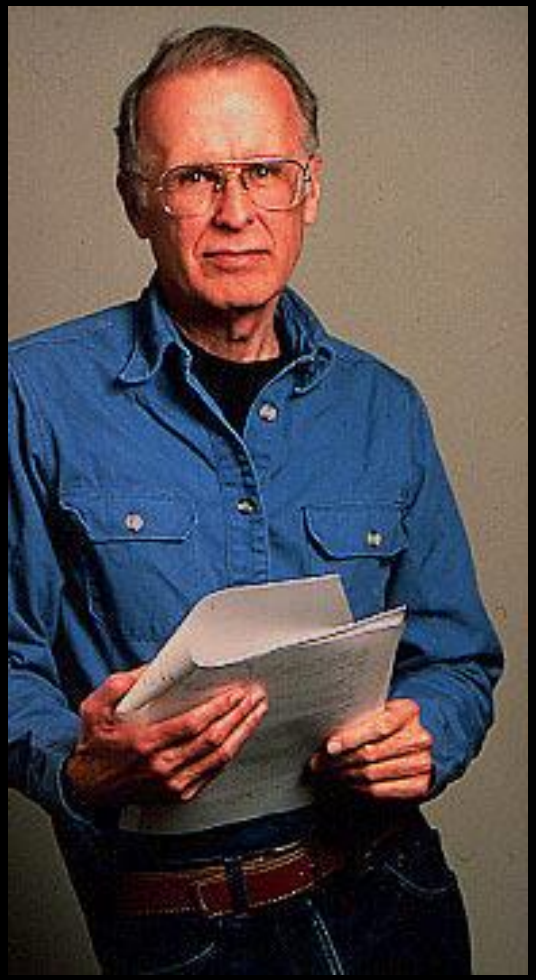
The gaps in the numbering within each category correspond to subroutines which have become obsolete.

Quality Numerical Software

- Should be:
  - Numerically stable, with measures of quality of solution
  - Reliable and robust
  - Accompanied by test software
  - Useful and user friendly with example programs
  - Fully documented
  - Portable
  - Efficient

John Backus

1924 - 2007



Best regards, Walter
John Backus

Programmer's
Reference Manual
October 15, 1956

THE FORTRAN AUTOMATIC CODING SYSTEM FOR THE IBM 704 EDPM®

This manual supersedes all earlier information about the FORTRAN system. It describes the system which will be made available during late 1956, and is intended to permit planning and FORTRAN coding in advance of that time. An Introductory Programmer's Manual and an Operator's Manual will also be issued.

APPLIED SCIENCE DIVISION
AND PROGRAMMING RESEARCH DEPT.
International Business Machines Corporation
590 Madison Ave., New York 22, N. Y.

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I. ZILLER

C ← FOR COMMENT / STATEMENT NUMBER (1–5)	CONTINUATION (6)	FORTRAN STATEMENT (7–72)	IDENTIFICATION (73–80)
C		PROGRAM FOR FINDING THE LARGEST VALUE	
C	X	ATTAINED BY A SET OF NUMBERS	
		DIMENSION A(999)	
		FREQUENCY 30(2,1,10), 5(100)	
		READ 1, N,.(A(I), I = 1,N)	
1		FORMAT (I3/(12F6.2))	
		BIGA = A(1)	
5		DO 20 I = 2,N	
30		IF (BIGA-A(I)) 10,20,20	
10		BIGA = A(I)	
20		CONTINUE	
		PRINT 2, N, BIGA	
2		FORMAT (22H1THE LARGEST OF THESE I3, 12H NUMBERS IS F7.2)	
		STOP 77777	

Fortran

- Fortran lives on – now Fortran 2003
- Fortran 2008 under discussion

Thank you John for all your work on the Fortran standard.

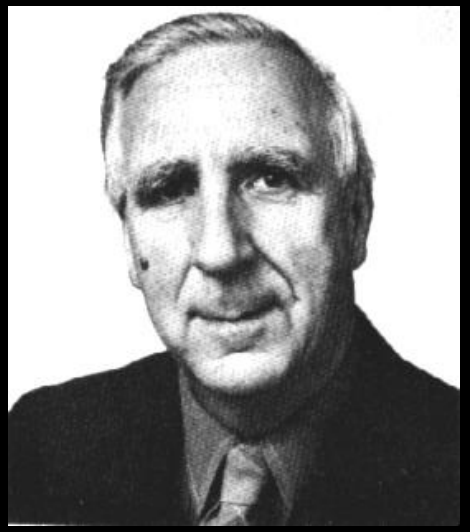
18 years on ISO committee, 10 as convenor

Language Support

- Need more language support of the sort provided in Fortran 2003 and C99
  - Machine (or environment) parameters
  - IEEE arithmetic, such as directed rounding
  - Exception handling
  - Interval arithmetic
- See W Kahan, *How Futile are Mindless Assessments of Roundoff in Floating-Point Computation?* http://www.cs.berkeley.edu/~wkahan/

“I have little doubt that about 80 per cent. of all the results printed from the computer are in error to a much greater extent than the user would believe, ..."

Leslie Fox, IMA Bulletin, 1971



“Giving business people spreadsheets is like giving children circular saws.

The average spreadsheet programmer does little or no advance planning, has no idea whether his or her algorithms are correct … builds in few or no cross-checks, and does little or no testing.

It is a cast iron certainty that the vast majority of spreadsheets contain errors”

Jack Schofield, The Guardian, 2003

NATIONAL PHYSICAL LABORATORY

Notes on Applied Science
No. 32

Rounding Errors in Algebraic Processes

by
J. H. WILKINSON, M.A., Sc.D.

LONDON
HER MAJESTY'S STATIONERY OFFICE
1963

N. J. Higham. *Accuracy and Stability of Numerical Algorithms*. SIAM, Philadelphia, PA, USA, second edition, 2002.

“Since the use of the punched-card equipment required the use of an operator, it encouraged user participation generally, and this was a distinctive feature of Pilot ACE operation

…

Speaking for myself I gained a great deal of experience from user participation, and it was this that led to my own conversion to backward error analysis.”

Wilkinson (1980) in *A History of Computing in the Twentieth Century*, Academic Press

Portability

- For portability, needed a model of floating point arithmetic
- IFIP/WG 2.5. B Ford et al. See: http://www.nsc.liu.se/~boein/ifip/projects/p1.txt
- W S Brown *A simple but realistic model of floating-point computation* ACM Trans. Math. Software,7, 445–480, 1981
- NAG: Chapter X02
- LAPACK: xLAMCH

John was a member of IFIP WG 2.5 for 25 years!

IEEE Arithmetic Formats

Format	Precision	Exponent	Approx Range	Approx precision (u)
Single	24 bits	8 bits	$10^{\pm 38}$	10^{-8}
Double	53 bits	11 bits	$10^{\pm 308}$	10^{-16}
Extended	≥ 64	≥ 15	$10^{\pm 4932}$	10^{-20}

W. Kahan's self-portrait

Handbook for Automatic Computation

Edited by

F. L. Bauer · A. S. Householder · F. W. J. Olver

H. Rutishauser † · K. Samelson · E. Stiefel

Volume II

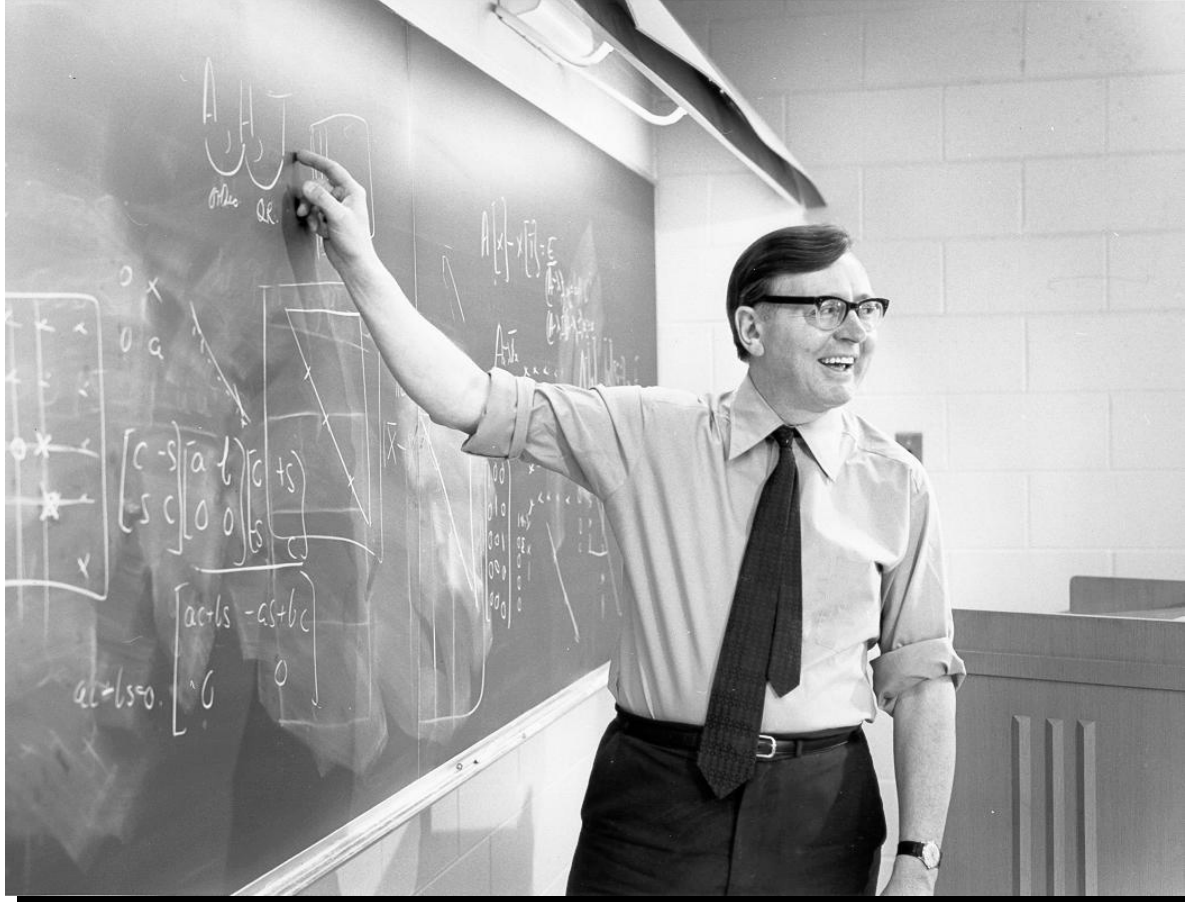
J. H. Wilkinson · C. Reinsch

Linear Algebra

Chief editor

F. L. Bauer

Springer-Verlag Berlin Heidelberg New York 1971



T. J. Dekker, W. Hoffmann; *Algol 60 procedures in numerical algebra part 2;* MC Tracts 23, Mathematisch Centrum, Amsterdam (1968)

Lecture Notes in Computer Science

Edited by G. Goos and J. Hartmanis

6

B. T. Smith · J. M. Boyle · J. J. Dongarra
B. S. Garbow · Y. Ikebe · V. C. Klema
C. B. Moler

Matrix Eigensystem Routines –
EISPACK Guide
Second Edition

Springer-Verlag
Berlin · Heidelberg · New York

LINPACK USERS' GUIDE

J.J. Dongarra C.B. Moler
J.R. Bunch G.W. Stewart

siam

Basic Linear Algebra Subprograms

- Level 1 BLAS, 1979
- Level 2 BLAS, 1988
  - Vector machines
- Level 3 BLAS, 1990
  - Hierarchical memory, shared memory parallel
- Dates are for TOMS publication

Blas Festival 2009

English | Gàidhlig

- welcome
- newsletter
- news
- about blas
- gallery
- contact us
- links

mailing list

Subscribe to our mailing list for information on this and future festivals...

tickets

Purchase tickets for all events at thebooth.co.uk or by contacting the venue...

News Feed

Celebrating the Highlands 4th - 12th September 2009

Welcome to the Blas Festival which celebrates the culture of the Scottish Highlands through music and language. Devised by The Highland Council in partnership with Fèisean nan Gàidheal and the Promoters Arts Network, Blas is now in its fourth year.

We are proud to announce that this year's festival which ran from the 5th-13th September 2008 was our most successful yet. In just our fourth year we broke our records for attendances and sell out shows. Congratulations to the promoters, communities, artists and all those who work for Blas in making it such a success.

We have a number of interesting developments in the pipeline which will ensure the Blas Festival remains a great 'homecoming party' for people who love Scottish culture.

This week we will be announcing our successful 2008 figures and we will soon be announcing our programme for 2009!

Check back with us for more news and updates soon!

Latest News

Ceòlraidh is a perfect case for Faculty of Advocates
12 Sep 2008

Leading International Music Artistes Give Blas Exclusive Taste of New Album
07 Sep 2008

Blas Offers Role Model for Festival Delivery
05 Sep 2008

Budget Car Hire

Blas Preferred Car Hire Partner

Homecoming Scotland 2009

homecomingscotland2009.com

John Francis (Mr *QR*)


ARGYLE STREET
blas
Lunch from £4.95
Soup & a Roll £4.95
2 course dinner £11.95
early evening dinner menu from 5 til 7
Dinner for 2 from £20
Tue to Thursday Main course & wine
Sunday Brunch Menu from £5.95
Teas, Coffee & Home Baking
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cafe restaurant bar
Teas
Coffees
Home Baking
Lunch &
Dinner
Malt Whisky
Scottish Ales
blas
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Scottish
Tapas from
£2.50 a bowl
Lunch
From £ 3.50
Dinner
£ 8.95 ~ £18.00
blas

Discussion of linear equation solvers on the Pilot ACE

"An interesting feature of the codes is that they made a very intensive use of subroutines; the addition of two vectors, multiplication of a vector by a scalar, inner products, etc., were all coded this way."

Wilkinson, 1980

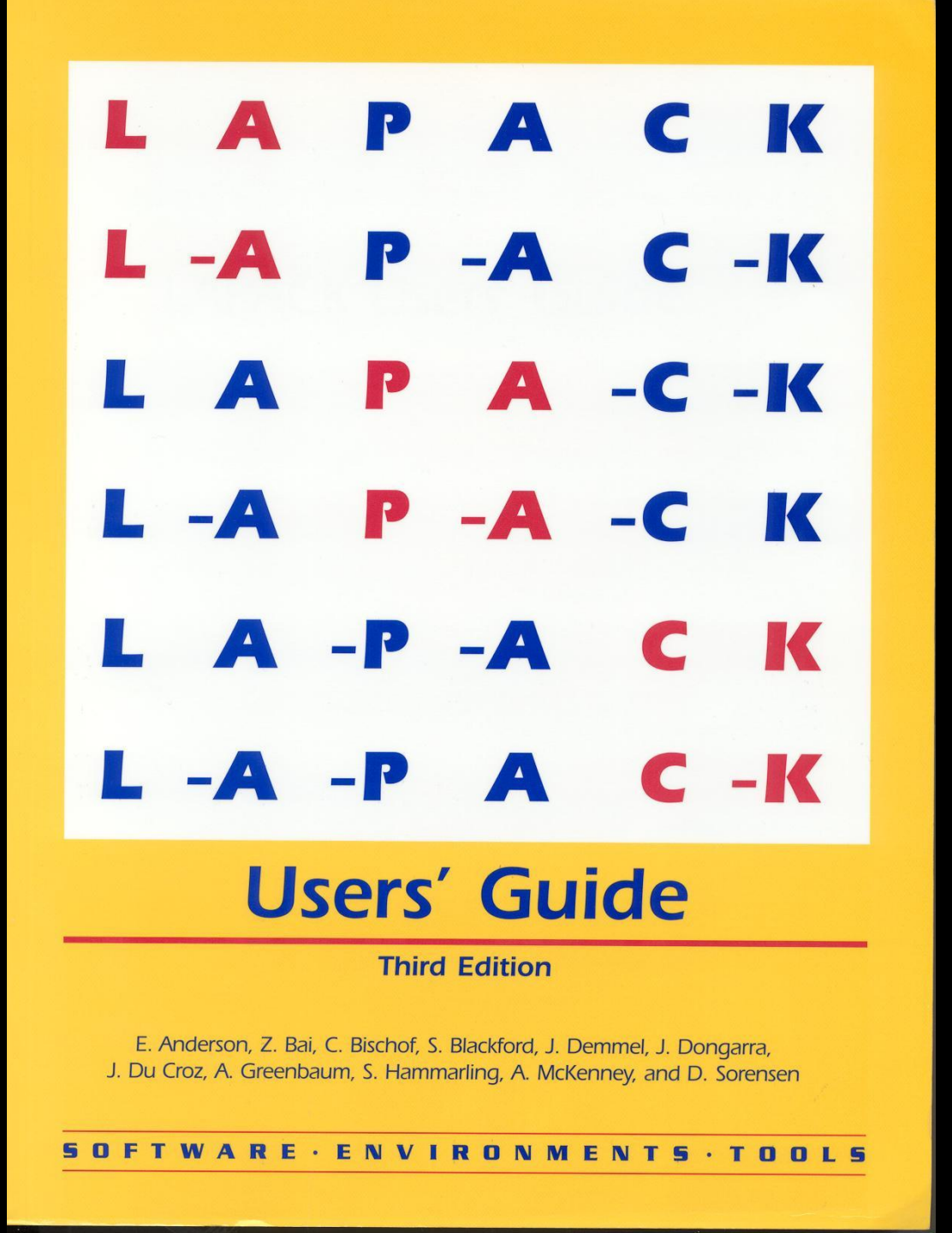
The History of Computing in the 20th Century.

Efficient Use of Data

"Since all machines have stores of finite size often divided up into high speed and auxiliary sections, storage considerations often have a vitally important part to play."

Wilkinson, MTAC, 1955

Emphasis on error and condition estimates, as well as efficiency




LAPACK

LAPACK95 Users' Guide

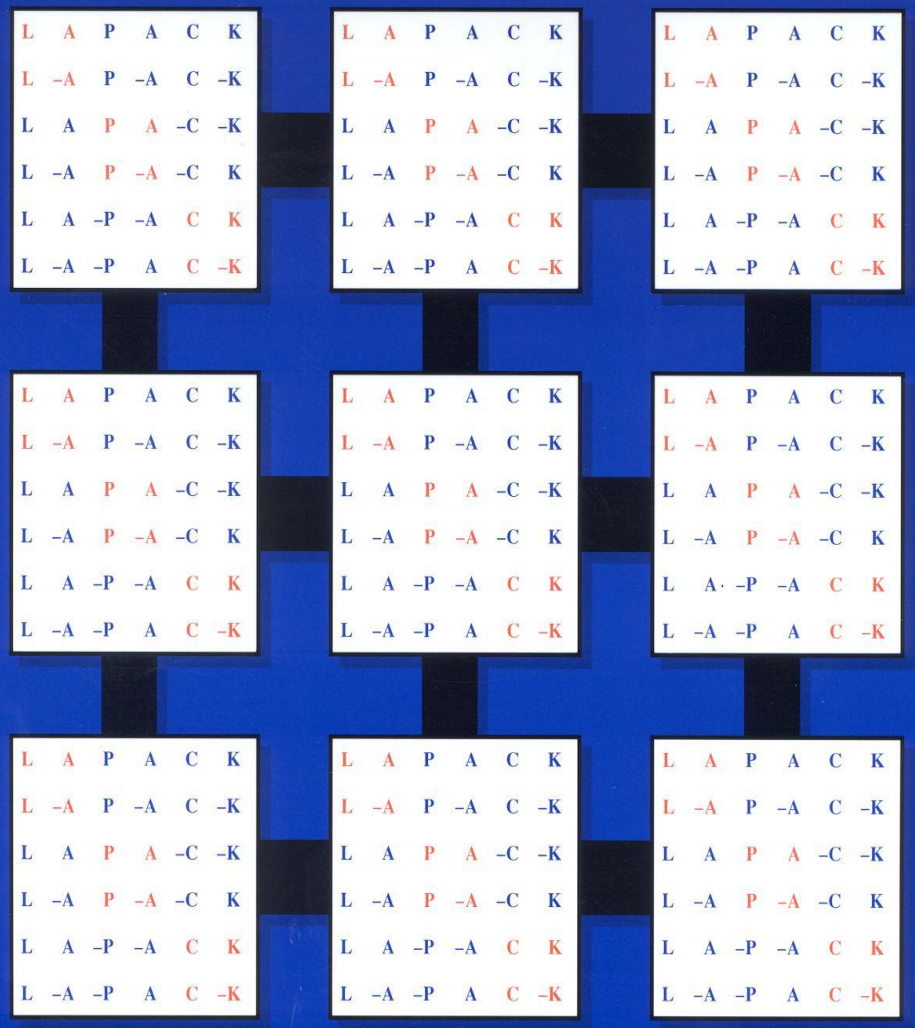
V. A. Barker, L. S. Blackford, J. Dongarra,
J. Du Croz, S. Hammarling, M. Marinova,
J. Waśniewski, and P. Yalamov

siam

SOFTWARE · ENVIRONMENTS · TOOLS

ScaLAPACK Users' Guide

L. S. Blackford · J. Choi · A. Cleary · E. D'Azevedo
J. Demmel · I. Dhillon · J. Dongarra · S. Hammarling
G. Henry · A. Petitet · K. Stanley · D. Walker · R. C. Whaley



Software Code Sizes

- NAG Fortran Library, Mark 21
  - Source: **28.3 Mb**
  - Stringent test programs: **42.1 Mb**
  - Example programs: **4.4 Mb**
  - XML documentation: **136 Mb**
- LAPACK 3.0
  - Source: **12.1 Mb**
  - Testing: **10.9 Mb**
  - Timing: **6.5 Mb**
  - Users' Guide: **407 pages**

Measures of Solution Quality

DGESVX is an 'expert' driver for solving $AX = B$

`DGESVX(...,RCOND,FERR,BERR,WORK,...,INFO)`

`RCOND` : Estimate of $1/\kappa(A)$

`FERR(j)`: Estimated forward error for X_j

`BERR(j)`: Componentwise relative backward error for X_j

(smallest relative change in any element of A and B

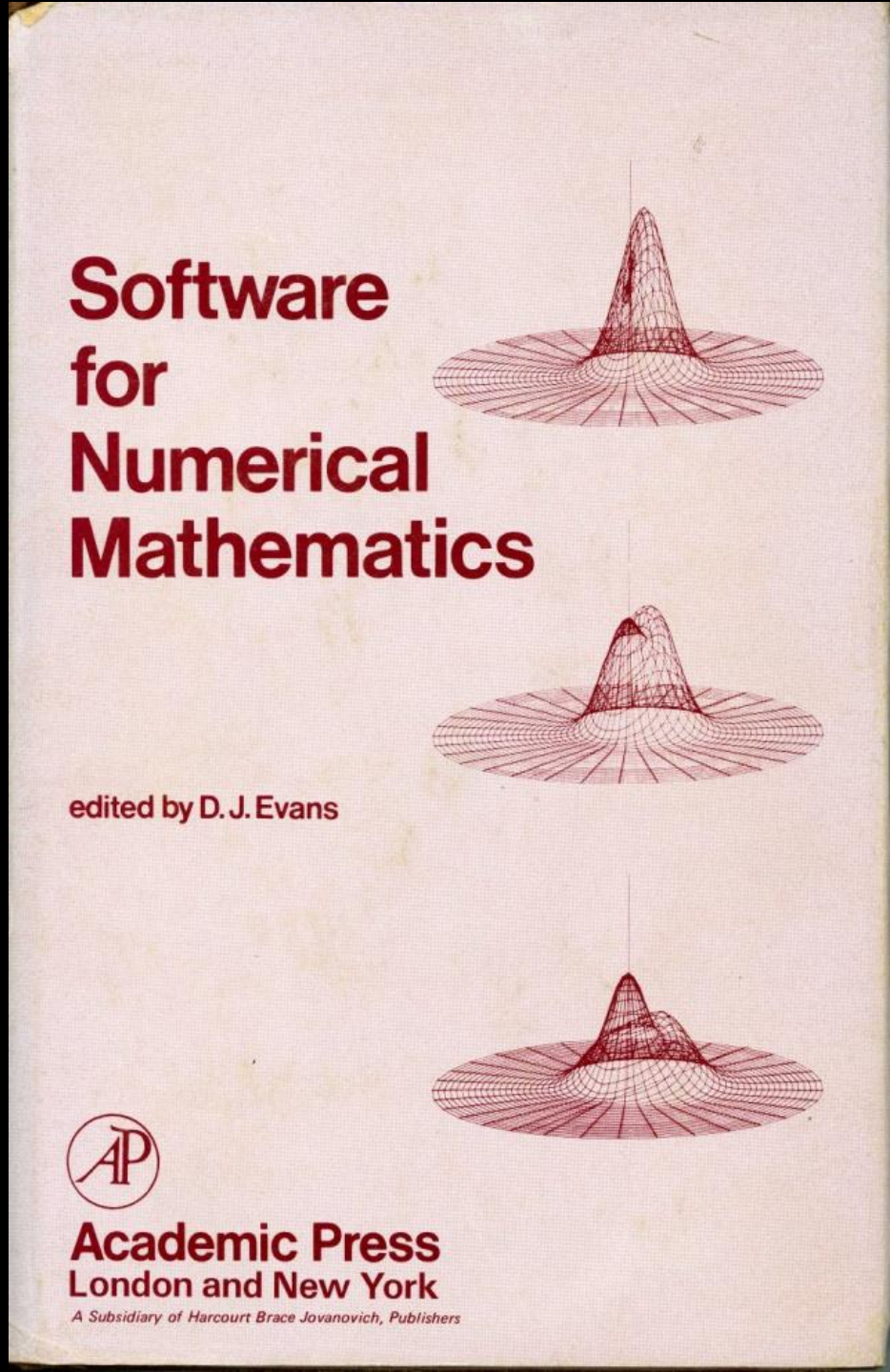
that makes X_j an exact solution)

`WORK(1)`: Reciprocal of pivot growth factor $(1/g)$

`INFO` : > 0 if A is singular or nearly singular

Proceedings of IMA Conference, Loughborough, 1973

Published 1974



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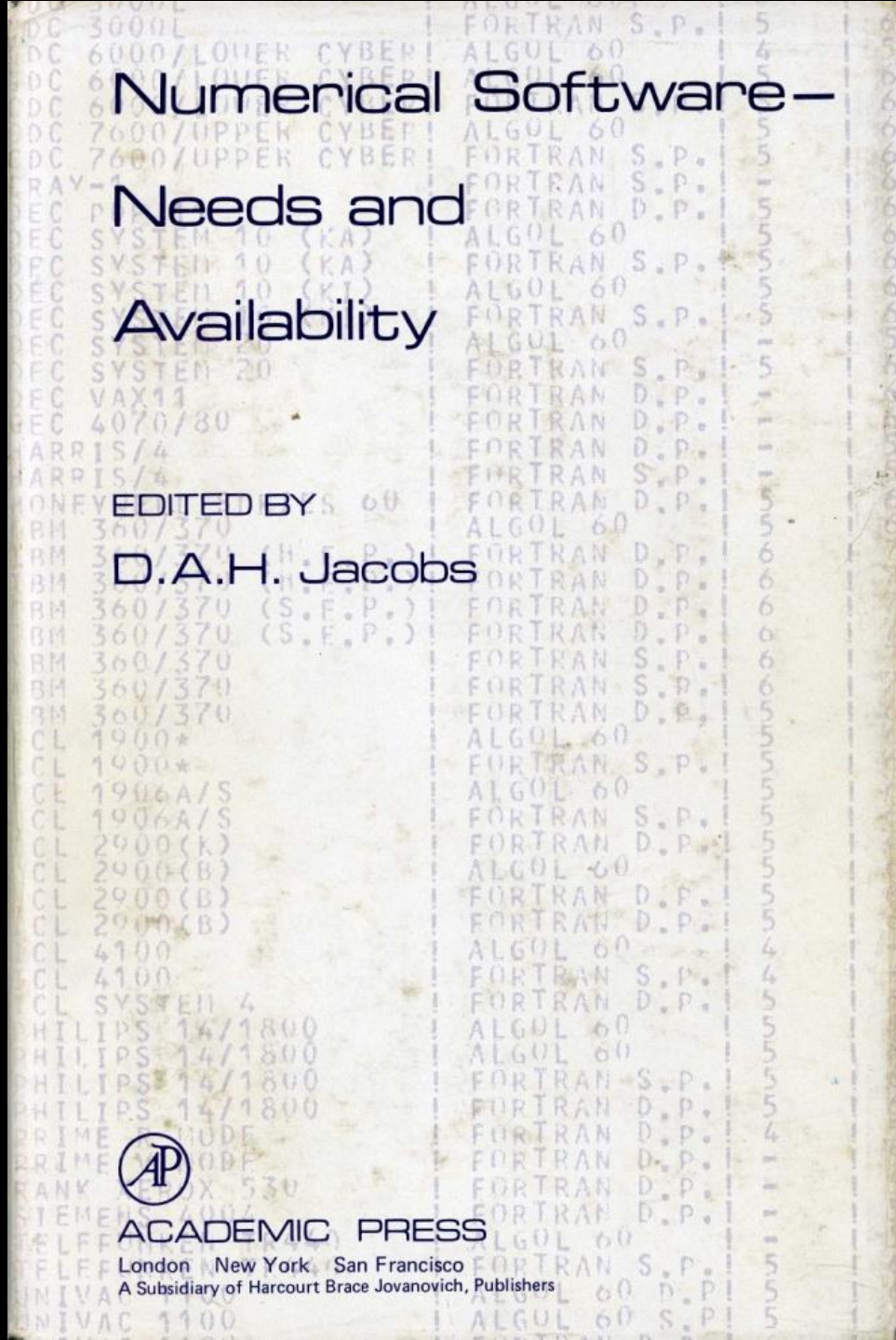
Proceedings of IMA Conference, Sussex 1977

Published 1978



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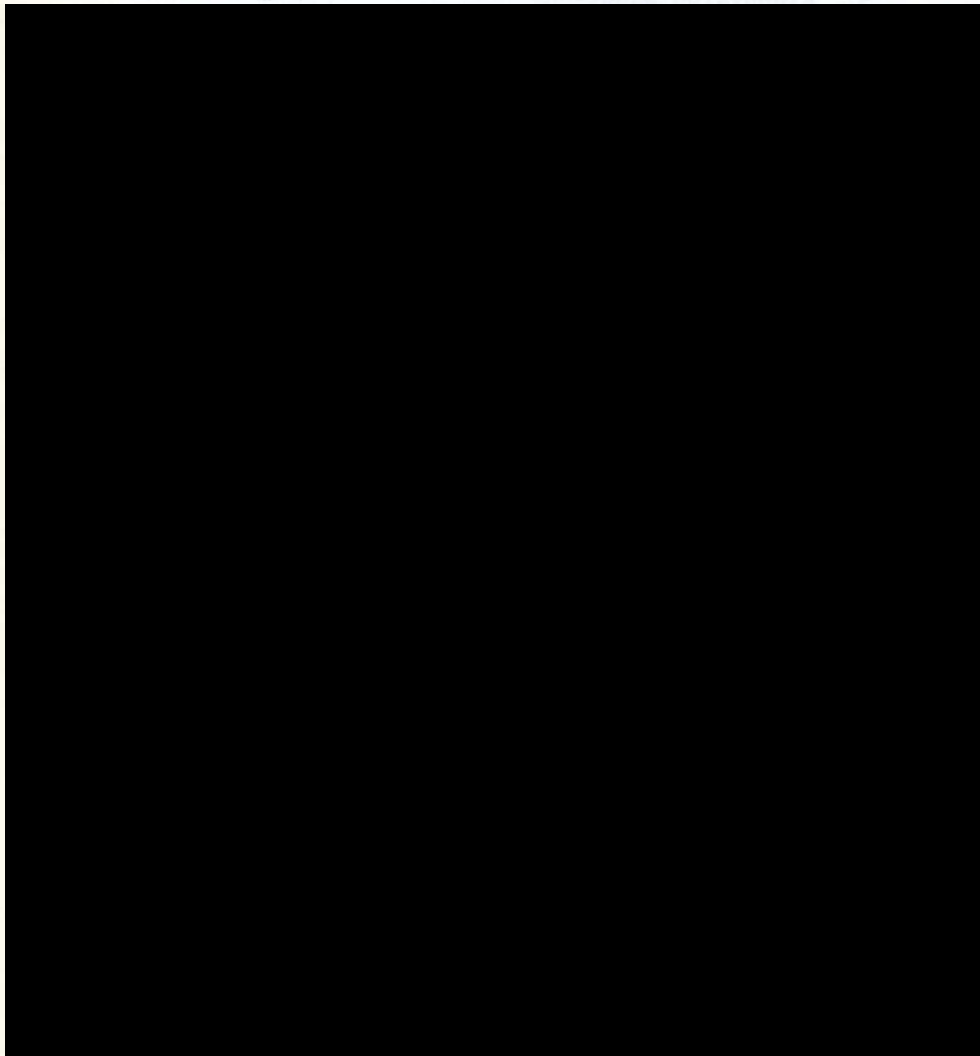
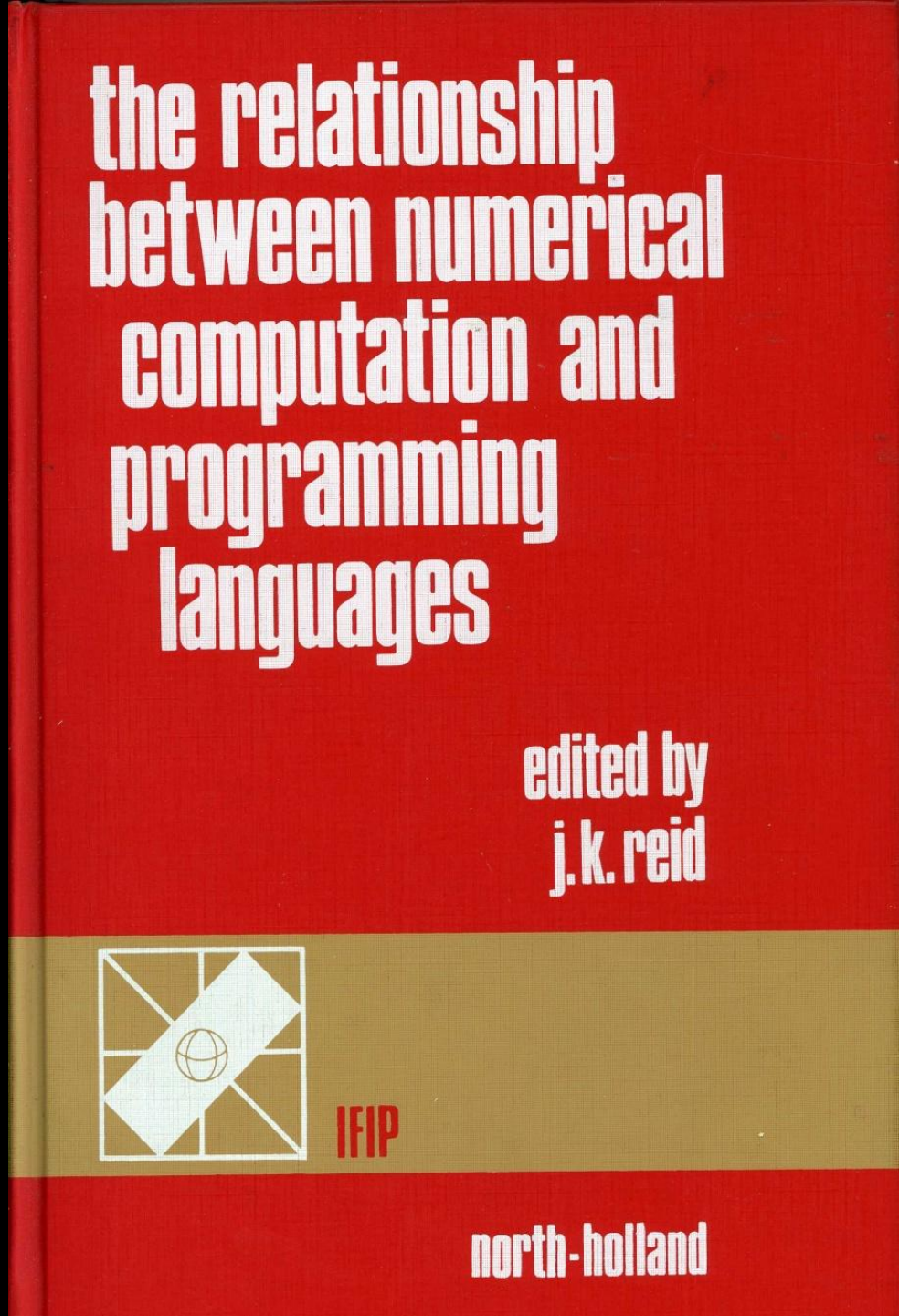


Proceedings of IFIP Conference, Boulder 1981

Published 1982

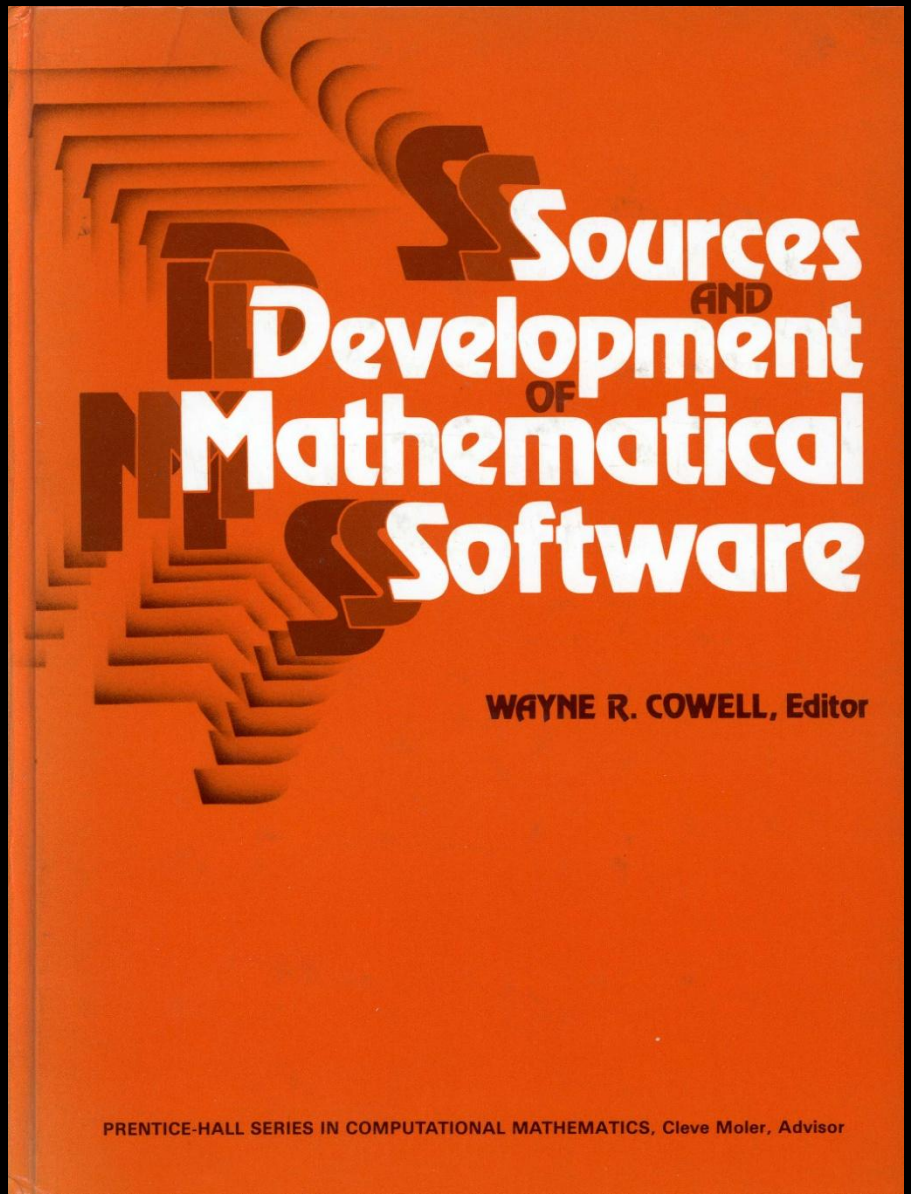
Included “Floating-point Parameters, Models and Standards by Jim Cody



Jim Cody in 1969

Sadly passed away
on June 24th, 2009

State of Libraries and Packages in 1984



Articles on:

- Observations on Mathematical Software Effort (Cody)
- LINPACK (Dongarra, Stewart)
- FUNPACK (Cody)
- EISPACK (Dongarra, Moler)
- MINPACK (Moré, Sorensen, Garbow, Hillstrom)
- Software for ODEs (Shampine, Watts)

... (cont'd)

- Sources of Information on Quadrature Software (Kahaner)
- A Survey of Sparse Matrix Software (Duff)
- Mathematical Software for Elliptic Boundary Value Problems (Boisvert, Sweet)
- The IMSL Library (Aird)
- The SLATEC Common Mathematical Library (Buzbee)

... (cont'd)

- The Boeing Mathematical Software Library (Erisman, Neves, Philips)
- The PORT Mathematical Subroutine Library (Fox)
- The Evolving NAG Library Service (Ford, Pool)
- ----------
- HSL

Today

- BCSLIB, IMSL, HSL and NAG are all alive
- A number of the PACKs are still available; LAPACK is probably the most active (but needs more funding)

- PETSc
- Trilinos (maintained repository), ...

Big Challenge for the Future

- Multicore and hybrid chips
- Dongarra: “There is no Moore’s law for software”

- See the final talk by Jack Dongarra