Fortran in the 21st Century
Presentation to BCS Wolverhampton Branch
Peter Crouch, Chairman BCS Fortran Specialist Group
Date: 27th January 2011
My Background


1993  Joined the British Computer Society

1997 – 2002  Chairman of the BCS Birmingham Branch

2002 – 2011  Chairman of the BCS Fortran Specialist Group
Commodore PET from late 1970s on which I learned to program in BASIC
Apple II system from early 1980s on which I learned to use Pascal and Fortran
<table>
<thead>
<tr>
<th>Year</th>
<th>Event</th>
</tr>
</thead>
<tbody>
<tr>
<td>1954</td>
<td>Development work starts in IBM</td>
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<tr>
<td>1957</td>
<td>IBM release a Fortran compiler for the IBM 704</td>
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<td>1958</td>
<td>IBM release Fortran II, with subroutines and blank common</td>
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<td>1960</td>
<td>Philco release ALTAC, a Fortran II look-alike</td>
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<tr>
<td>1961</td>
<td>IBM have eight different compilers (for the 709, 650, 1620 and 7090) and publish a guide to language variations between them</td>
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<tr>
<td>1961</td>
<td>Univac release Fortran I for the SS80, the first compiler called ‘Fortran’ for a non-IBM machine</td>
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</table>
Fortran Pioneers, lead by John Backus: 25 years on, June 1982

Pioneer Day Banquet, June 1982

The first Fortran Standard 1962-1966

<table>
<thead>
<tr>
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<tbody>
<tr>
<td>1962</td>
<td>Work on an ASA standard begins in order to promote consistency and enable portability</td>
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<tr>
<td>1962</td>
<td>IBM release Fortran IV for the 7030, 7090 and 7094; this removes some of the machine dependencies</td>
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<tr>
<td>1963</td>
<td>Most major US vendors have Fortran systems, either Fortran II or, increasingly, Fortran IV</td>
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<tr>
<td>1964</td>
<td>Technical work on the standard is complete. It is essentially a common subset of vendors’ offerings</td>
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<tr>
<td>1965</td>
<td>ICT have Fortran IV on the 1900 and English Electric have Egtran on the KDF9</td>
</tr>
<tr>
<td>1966</td>
<td>The ASA/USASI standard is published Clarifications are published in 1969 and 1971 (The US standard is reproduced as an ISO standard in 1972)</td>
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</tbody>
</table>
The first US Standard X3.9-1966 (FORTRAN 66)
FORTRAN IV or 66 example code

C       THE TPK ALGORITHM
C       FORTRAN IV OR 66 STYLE
DIMENSION A(11)
FUN(T) = SQRT(ABS(T)) + 5.)*T**3

READ (5,1) A
1   FORMAT(5F10.2)
DO 10 J = 1, 11
   I = 11 - J
   Y = FUN(A(I+1))
   IF (400.0-Y) 4, 8, 8
4      WRITE (6,5) I
5      FORMAT(I10, 10H TOO LARGE)
   GO TO 10
8      WRITE(6,9) I, Y
   FORMAT(I10, F12.6)
10     CONTINUE
STOP
END
The Fortran Specialist Group is established: 1970

FSG Minutes of 6 January 1970:

The objectives of the group were formally agreed to be:

(a) to form a focus in the United Kingdom for work concerned with establishing and maintaining FORTRAN standards.

(b) to work in association with national and international standardisation bodies.

FSG Minutes of 5 April 1976:

4. Revision of objectives

Following further discussion, the wording of the proposed revised objectives now becomes "To undertake activities associated with any aspects of Fortran".

It is intended to present this for approval at the next Specialist Groups meeting.

January 1970
- Analyse existing standard
- Comparison of existing compilers
- Extension to Fortran

April 1970
- Extensions to ASI Fortran IV
- Adaptation to conversational use
- Fortran on small machines

April 1971
- Free format
- Mini computers
- Diagnostics
- Extensions

1975
- FORTREV (draft Fortran 77) review

April 1976
- Preprocessors
- Group Promotion & Information

December 1976
- Review Codasyl FDBMLC JOD
FSG Activities 1970-1980

• FSG hold typically four to six meetings per year, mostly discussing working party progress, applications, software tools, programming techniques and, from late 1971, Fortran standards developments

• First contact with X3J3 members 1971

• FSG get on X3J3 mailing list and two-way flow of information and opinion starts

• FSG members attend occasional X3J3 meetings in the US

• Presentations are made at conferences and workshops, e.g. Datafair 73, 75 and 77 and a Fortran Forum in London in 1978 with six US members of X3J3 as speakers
FORTRAN 77: Principal changes

- type CHARACTER
- IMPLICIT, PARAMETER, SAVE
- block IF
- ENTRY
- INQUIRE
- new intrinsic functions
- many detailed extensions to existing statements
- real and double precision DO index
- removal of Hollerith constants and data
The second US Standard X3.9-1978 (FORTRAN 77)
PROGRAM TPK
C       THE TPK ALGORITHM
C       FORTRAN 77 STYLE
REAL A(0:10)
READ (5,*) A
DO 10 I = 10, 0, -1
   Y = FUN(A(I))
   IF (Y .LT. 400) THEN
      WRITE(6,9) I,Y
   9 FORMAT(I10. F12.6)
   ELSE
      WRITE (6,5) I
   5 FORMAT(I10,' TOO LARGE')
ENDIF
10 CONTINUE
END

REAL FUNCTION FUN(T)
REAL T
FUN = SQRT(ABS(T)) + 5.0*T**3
END
MIL-STD-1753 1978: US DoD supplement to FORTRAN 77

IMPLICIT NONE
INCLUDE
END DO
DO WHILE

Additional functions for bit manipulation
FSG Activities 1981-1993

- FSG thrives, continuing in the same mode
- Fortran Forums are held in London (4) and Edinburgh (2), sometimes with visiting US speakers
- Some meetings are held outside London: Blacknest, Coventry, Jodrell Bank, Oxford, Reading, Rutherford Lab, Salford
- An experimental subgroup meeting is held in Glasgow as part of a drive for every Specialist Group to have meetings in Scotland
- Some FSG members become members of X3J3 and/or WG5 and attend regularly; others attend occasionally; the UK plays a significant part in development of Fortran 90
Development of Fortran 90

• Originally scheduled for completion in 1982

• Renamed Fortran 8X, then Fortran 88 and finally completed in 1990 after rancorous discussions and attempts by some US vendors to derail the entire project

• Some US organizations attempt to retain Fortran 77 alongside Fortran 90

• See “The Fortran (not the foresight) saga: the light and the dark” by Brian Meek and “The Standards Hiatus” by Miles Ellis and Lawrie Schonfelder, both linked from www.fortran.bcs.org/2007/jubileeprog.php
Fortran 90: Principal changes

- Free form source form
- Many minor modernizations and removal of arbitrary restrictions
- Whole array operations
- Facilities for modular data and procedure definitions
- Improved control over numerical computation
- Parameterized intrinsic types
- User-defined data types
- Pointers
- Some features deemed obsolescent – to allow for future deletion
- **Still retaining compatibility for Fortran 77 programs!!**
ISO/IEC 1539:1991 (Fortran 90)
First Fortran 90 Compiler

• Numerical Algorithms Group (NAG), based in Oxford, announce the world’s first Fortran 90 compiler in June 1991

• The FSG nominate NAG for a BCS Excellence award; NAG are awarded a BCS medal
PROGRAM TPK
! The TPK Algorithm
! Fortran 90 style
IMPLICIT NONE
INTEGER :: I
REAL :: Y
REAL, DIMENSION(0:10) :: A
READ (*,*) A
DO I = 10, 0, -1
! Backwards
  Y = FUN(A(I))
  IF ( Y < 400.0 ) THEN
    WRITE(*,*) I, Y
  ELSE
    WRITE(*,*) I, ' Too large'
  END IF
END DO
END PROGRAM TPK

CONTAINS
! Local function
FUNCTION FUN(T)
  REAL :: FUN
  REAL, INTENT(IN) :: T
  FUN = SQRT(ABS(T)) + 5.0*T**3
END FUNCTION FUN
END PROGRAM TPK
The F language: a regular subset of Fortran 90

• Specified by a small group of experts involved in the development of Fortran 90 as a language that was highly regular in syntax and safe in use

• Intended to be easy to learn and reliable to use while retaining the powerful numerical features of Fortran 90

• Comprises the modern features introduced in Fortran 90 without the older, unsafe features of earlier versions of the language

module Functions

public :: fun

contains

  function fun(t) result (r)
    real, intent(in) :: t
    real :: r
    r = sqrt(abs(t)) + 5.0*t**3
  end function fun

end module Functions

All example programs copied from Bo Einarsson's website at www.nsc.liu.se/~boein/f77to90/a7.html#introduction
program TPK
  ! The TPK Algorithm
  ! F style

use Functions

integer  :: i
real     :: y
real, dimension(0:10) :: a
read *, a
do i = 10, 0, -1            ! Backwards
  y = fun(a(i))
  if ( y < 400.0 ) then
    print *, i, y
  else
    print *, i, " Too large"
  end if
end do
end program TPK
Fortran 95: Principal changes

Part 1:

- FORALL
- PURE and ELEMENTAL procedures
- Initialization for pointers and for structures
- Designation of some older, duplicated features as ‘obsolescent’
- *Deletion of REAL and DP DO variables, PAUSE, ASSIGN and assigned GO TO, H edit descriptor*

Part 2:

- Varying length strings
FSG Activities 1993-2001

- Attendances wilt with the advent of the internet

- The FSG debates winding itself up but decides against

- In 1994, taking advantage of X3J3 and WG5 meetings in the UK, well-attended forums are held in Edinburgh, London and Oxford – but:

  - a nadir is reached when the 1995 AGM is postponed because of a rail strike and the 1996 AGM is postponed due to rooms being double-booked; not everyone gets to know in time
  - It is decided to hold only annual meetings plus special events

- NAG hold very successful ‘Fortran Futures 96’ and ‘Fortran Futures 98’ conferences “in association with the FSG”
Fortran 2003: Principal changes

- Parameterized derived types
- Object oriented programming support
- I/O enhancements, including stream access and asynchronous transfers
- Support for IEEE arithmetic and exception handling
- Standardised interoperability with C
- Support for ‘international usage’
- ASSOCIATE construct
- Data manipulation enhancements: allocatable components, etc
- Procedure pointers
- Scoping enhancements
- Access to command line arguments, environmental variables

INTERNATIONAL STANDARD

ISO/IEC 1539-1

Second edition
2004-11-15

Information technology — Programming languages — Fortran —
Part 1:
Base language

Reference number
ISO/IEC 1539-1:2004(E)
Fortran 2003: Implementation Problems

- Fortran 2003 turns out to be far more difficult to implement than had been foreseen

- Cray release the first full compiler, for some of their hardware, in December 2009 - six years after completion of the technical definition

- In 2010 IBM are the second vendor to release a full compiler

- Some suppliers let it be known that they plan to implement all of Fortran 2003 only if explicitly required by their customers
Coarrays as an extension for parallel processing

Submodules to reduce compilation cascades

Enhancements to aid optimisation

Data enhancements including long integers, maximum array rank increased to 15, available kinds, hyperbolic and other functions

I/O enhancements including getting unique unit numbers, new edit descriptors

New BLOCK construct with declarations

Bit manipulation procedures

Execution of command shell commands
<table>
<thead>
<tr>
<th>Year</th>
<th>Standard</th>
<th>Description</th>
<th>Pages</th>
</tr>
</thead>
<tbody>
<tr>
<td>1966</td>
<td>ANSI X3.9-66 (FORTRAN 66)</td>
<td>first programming language standard</td>
<td>39 pages</td>
</tr>
<tr>
<td>1978</td>
<td>ANSI X3.9-78 (FORTRAN 77)</td>
<td>also published as ISO 1539:1980</td>
<td>243 pages</td>
</tr>
<tr>
<td>1991</td>
<td>ISO/IEC 1539:1991 (Fortran 90)</td>
<td>major revision</td>
<td>294 pages</td>
</tr>
<tr>
<td>1997</td>
<td>ISO/IEC 1539-1:1997 (Fortran 95)</td>
<td>minor revision</td>
<td>356 pages</td>
</tr>
<tr>
<td>2010</td>
<td>ISO/IEC 1539-1:2010 (Fortran 2008)</td>
<td>major revision</td>
<td>603 pages</td>
</tr>
</tbody>
</table>
Compiler support for Fortran 2003 & 2008 Standards

- Table first published April 2007, revised every 3 months
- Section on Fortran 2008 features added August 2009
- Information on 8 compilers currently available

- ACM Fortran Forum magazine – latest version
- Fortranplus website – previous version
  www.fortranplus.co.uk/resources/fortran_2003_2008_compiler_support.pdf

- Information courtesy of Ian Chivers and Jane Sleightholme,
  www.fortranplus.co.uk
FSG Activities 2002-2010

The FSG is revivified:

- In 2002 a Forum is held to discuss UK requirements for inclusion in Fortran 2003
- Also in 2002 a successful application is made to the BCS to support three FSG members (reduced to one member latterly) to attend WG5 meetings to help put the UK case on standards
- In 2007 a very successful full-day meeting is held with the CCS to mark the 50th anniversary of the release of the first Fortran compiler
- FSG members organize the 2007 WG5 meeting in BCS London offices and hold a reception for WG5 members
- In 2010 a successful meeting is held with the Institute of Physics to mark the 40th anniversary of the Fortran SG
'Fifty Years of Fortran' meeting
January 2007
Alex Stepanov, John Backus (1924-2007) and Paul McJones - February 2004
Some current application areas for Fortran

- **Weather forecasting and climate prediction**
- Analysis of seismic data for oil and gas exploration
- Financial analysis
- Vehicle crash simulation
- Analysis of data from space probes and satellites
- **Modelling of nuclear weapons** and **test ban verification**
- Computational fluid dynamics, the “**Numerical Wind Tunnel**”
NEC SX-8 supercomputer as used by UK Met Office
Fortran CFD program used in design of 1000 mph car - September 2010 issue of ITNOW
The CASTEP project: reflections on the first ten years

Keith Refson
STFC Rutherford Appleton Laboratory
Chilton, Didcot, OXON OX11 0QX

Presentation given to BCS Fortran SG on 30 Sep 2010 -
www.fortran.bcs.org/2010/agenda10.php#present
The CASTEP project: Materials Modelling by Quantum Mechanics

Fortran in Materials Modelling

Planewave
CASTEP PEtot
VASP PARATEC
PWscf Da Capo
Abinit CPMD
Qbox fhi98md
PWPAW SFHIngX
DOD-pw NWchem

Gaussian
CRYSTAL CP2K

Numerical
FHI-Aims SIESTA Dmol ADF-band

DFT
Ψ(r), n(r)

LAPW WIEN2k Fleur exciting Elk

http://www.psi-k.org/codes.shtml
CASTOR HPC Capability

HPC Capability: Peptide in water 1280 atoms
If you want to know more

Modern open source and free Fortran compilers are available from a number of sources as are online tutorials.

The Final Committee Draft of the Fortran 2008 standard is available from the WG5 website as document **N1830.pdf**. The technical content is identical to that of ISO/IEC 1539-1:2010.

Links to the above and more are available from the Resources page of the Fortran SG website at [www.fortran.bcs.org/resources.php](http://www.fortran.bcs.org/resources.php).
Further Information

FSG website
www.fortran.bcs.org/index.php

WG5 document archive
www.nag.co.uk/sc22wg5/

J3 document archive
www.j3-fortran.org/

Fortran and Fortran II history, including 1982 IBM film
www.softwarepreservation.org/projects/FORTRAN/
Acknowledgements

Many thanks to David Muxworthy for his presentation to the joint BCS/IoP meeting in June 2010 marking the 40th anniversary of the BCS Fortran Specialist Group. Many of the slides in this presentation are taken from it.

Other slides are based on parts of presentations given by Keith Refson and Ian Chivers and Jane Sleightholme following the FSG AGM in September 2010.

Thanks also to Paul McJones of the Computer History Museum, Mountain View, CA, for providing me with DVD versions of two IBM films and the 2004 photo of John Backus.

Finally I must thank all my colleagues in the Fortran Specialist Group for their assistance and encouragement during my time as Chairman.