Verification of Fortran Codes

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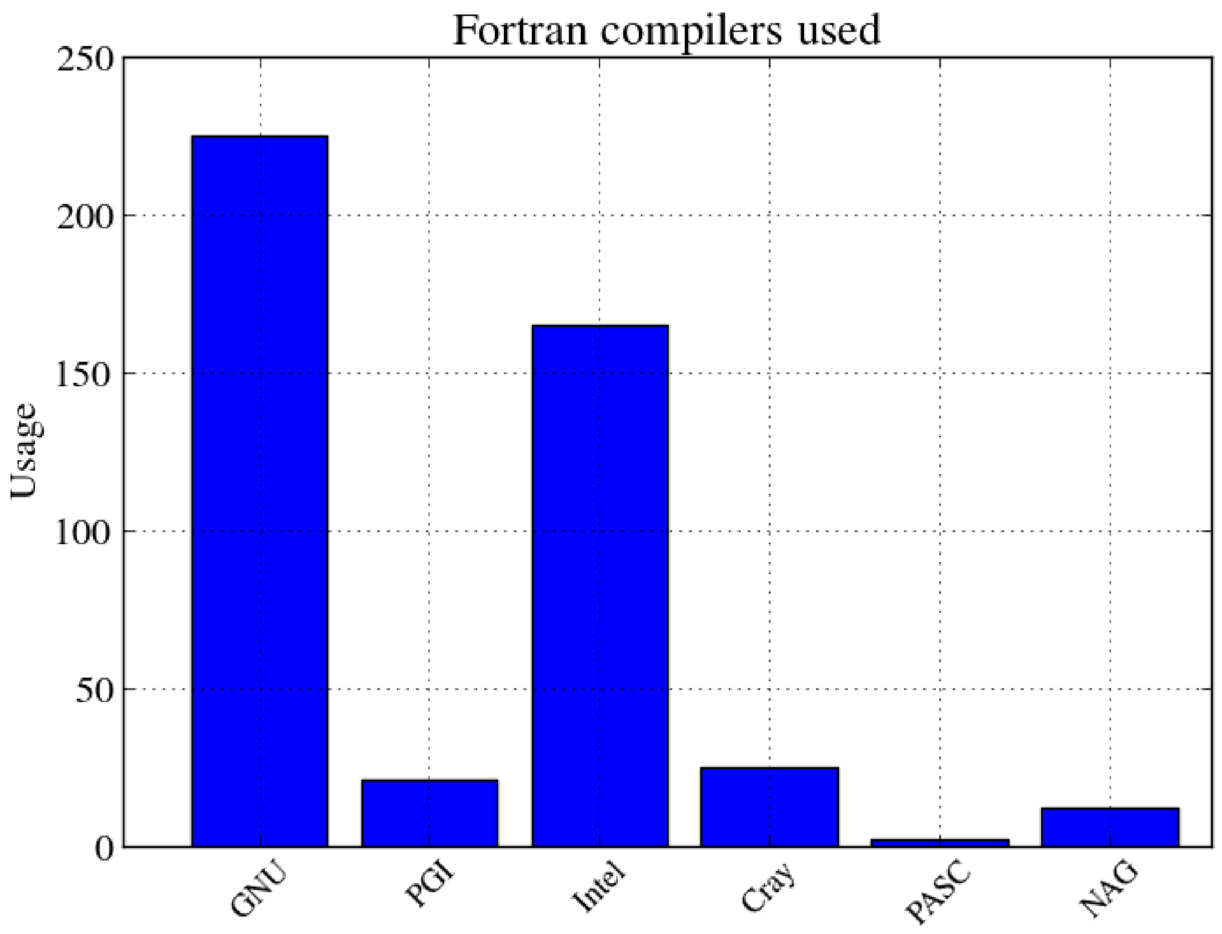
http://www.nag.co.uk/content/fortran-modernization-workshop

Fortran Compilers

- Compilers seem to be either high performant or very good at error checking;
- There is a spectrum in between and compilers fall somewhere in between;
- Clearly the GNU and Intel compilers are mostly used, but how good are they at error checking?



Verification Features of Fortran Compilers

- Compiler vendors either focus their efforts on performance or good verification features (or maybe neither);

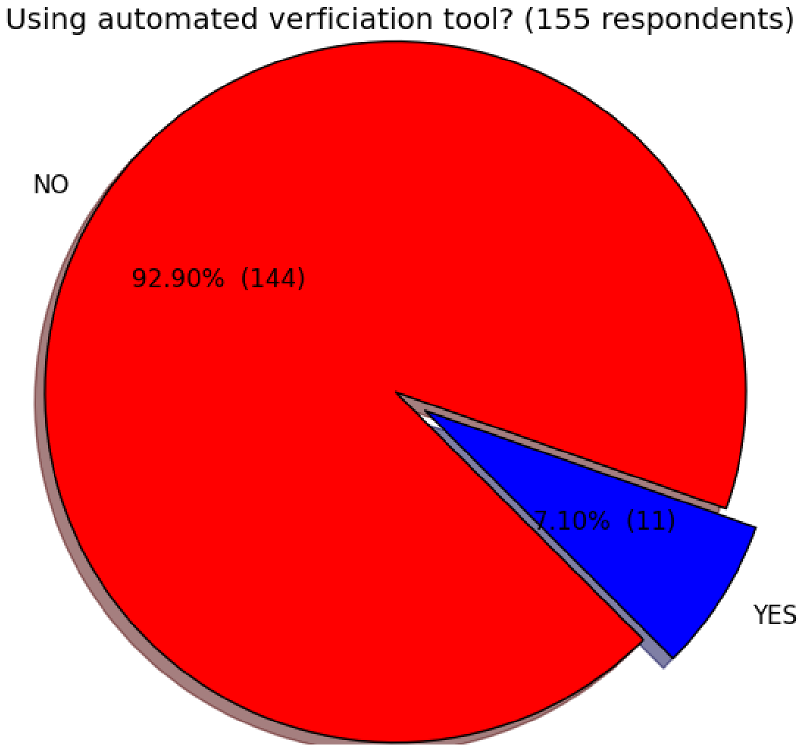
Run-time Error	Absoft	g95	gfortran	Intel	Lahey	NAG	Pathscale	PGI	Oracle
Percentage Passes [1]	34%	45%	53%	53%	92%	91%	38%	28%	42%
TFFT execution time with diagnostic switches (seconds)[2]	10	16	6	12	446	60		19	9

- The two most commonly used compilers, namely Intel and GNU Fortran, are only able to detect 53% of defects in the benchmark suite;
- The NAG compiler is able to capture 91% of defects in the benchmark suite.

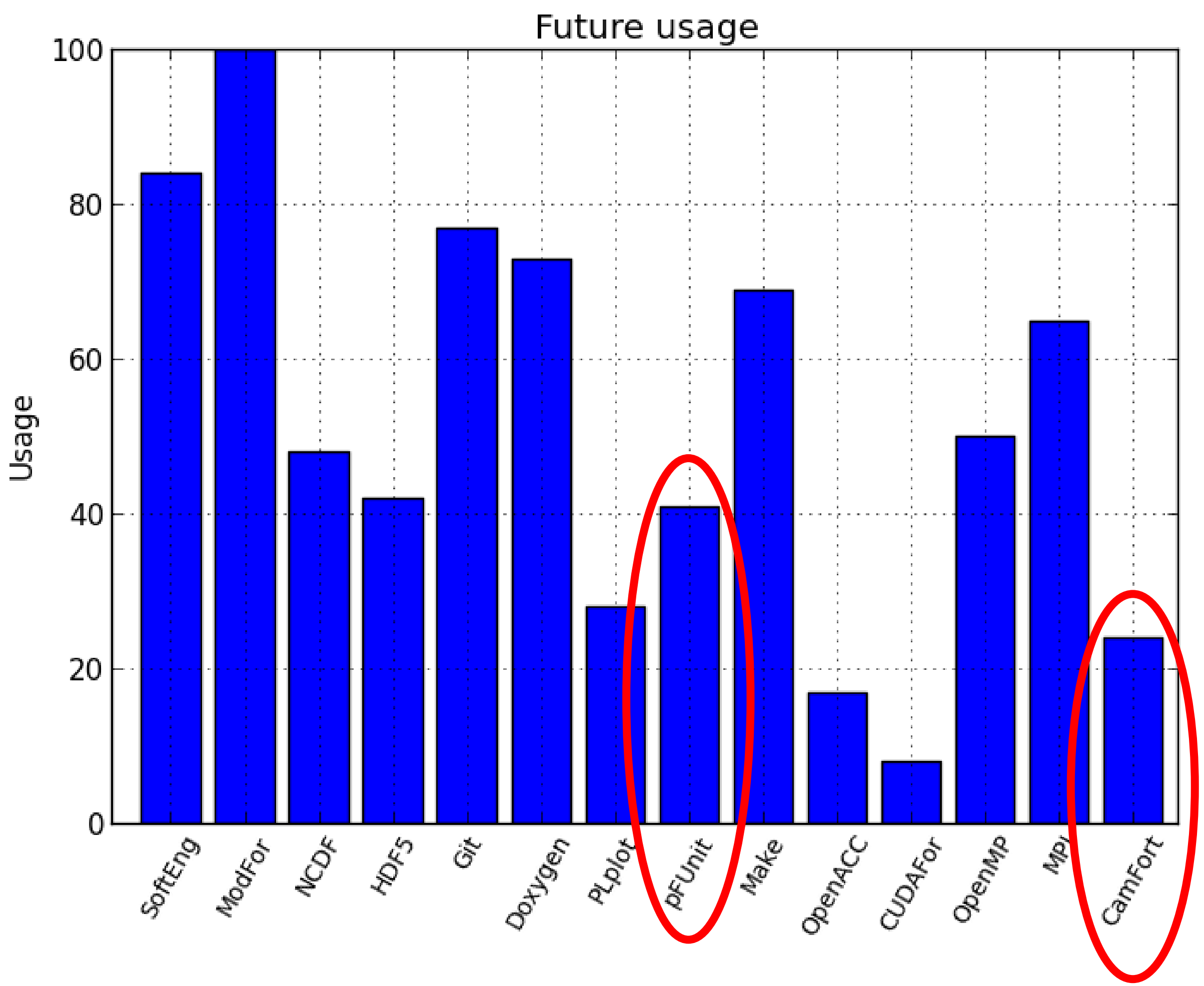
http://www.fortran.uk/fortran-compiler-comparisons-2015/intellinux-fortran-compiler-diagnostic-capabilities/

Usage of Verification Tools

- *Only 11 (7%) out of 155 Fortran developers are using verification tools;*
- Is there an over-reliance on compilers to detect defects? This certainly seems to be case;
- Advantage of verification tools is that they can detect bugs before a production run.



What Interests Fortran Programmers?



- There is anecdotal evidence to suggest that code verification is not considered important amongst Fortran programmers;
- This could obviously affect the quality of computational science codes.

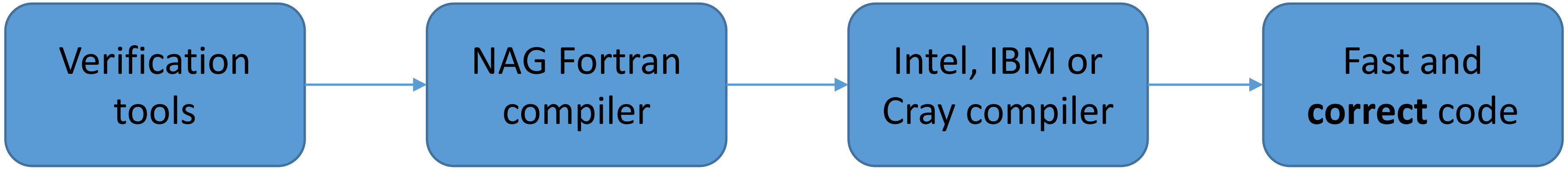
Fortran Verification Workflow (1)

- Computational scientists obviously want correct code as well as fast code. What is the answer?
- Use both error checking and high performance compilers in tandem with automated verification tools;
- Static analysis tools still have limitations so the code still requires runtime checks with a good error checking compiler, e.g. NAG;
- Unit tests should be built with the NAG compiler with optimisations switched off. Use the following compiler flags with the NAG compiler:

```
nagfor -C=all -C=undefined -info -O0 -g -gline
```

Fortran Verification Workflow (2)

- Integration tests should also be built with the NAG compiler with optimisations switched off;
- Once all tests have passed, then build with more performant compilers such as the Intel, Cray or IBM compilers.



Static analysis checks - CamFort, Forcheck, FPT

Rigorous standards checking and **runtime checks**

High performance compilers

Fortran Verification Tools

- CamFort [1];
- FPT [2];
- Forcheck [3];
- NAG Fortran compiler [4];
- pFUnit is a unit testing framework [5];
- I will only very briefly discuss FPT, Forcheck and the NAG Fortran compiler.

[1] https://github.com/camfort/camfort [2] http://www.simconglobal.com/ [3] http://www.forcheck.nl/
[4] https://www.nag.co.uk/nag-compiler [5] http://pfunit.sourceforge.net/

Fortran Array Bug

- Spot the bug below:

```
real, dimension(3) :: eng, aero
do i = 1, 3 ! 1 = port, 2 = centre, 3 = starboard
  aero = eng(i)
end do
! modern and correct version
aero(:) = eng(:)
```

- The FPT tool can detect the do loop bug.

Precision Bugs (1)

- The following code segments have bugs:

```
real(kind=REAL32) :: a, geom, v, g_p
a = geom * v ** (2/3) ! calculate surface area
g_p = 6.70711E-52

real(kind=REAL64) :: theta
real(kind=REAL32) :: x
x = 100.0_REAL64 * cos( theta )
```

Precision Bugs (2)

```
real(kind=REAL64) :: d
real(kind=REAL32) :: x, y
d = sqrt( x**2 + y**2 )
```

- Compilers are generally not good at spotting precision bugs;
- Compilers are not very good at detecting mixed precision bugs but the FPT and Forcheck tools can.

Forcheck Dummy Argument Checking

- Fortran code:

```
subroutine foo( a, b )
  real :: a
  real, optional :: b
  a = b**2 ! not checking to see if b is present
end subroutine foo
```

- Analysis output:

```
(file: arg_test.f90, line: 14)
B
**[610 E] optional dummy argument unconditionally used
```

Forcheck Dummy Argument Intent Checking

- Dummy arguments should always be scoped with the `intent` keyword;
- Command:

```
forchk -intent arg_test.f90
```

- Analysis output:

```
B
**[870 I] dummy argument has no INTENT attribute
         (INTENT(IN) could be specified)
```

Forcheck Actual Argument Checking

- Fortran code:

```
call foo( 1.0, b )
```

- Analysis output:

```
       7  call foo( 1.0, b )
(file: arg_test.f90, line: 7)
FOO, dummy argument no   1 (A)
**[602 E] invalid modification: actual argument is
constant or expression
```

Runtime Checking

- Static analysis checks are easy ways to detect obvious bugs but they are ultimately very conservative. When they say there is a bug, they are correct, i.e. do not give false positives;
- Static analysis tools are limited in what they can achieve particularly for large multi-scale multi-physics code where there can be variables that are defined in complex IF statements;
- This requires runtime checks to ultimately check for potential bugs with a comprehensive error checking compiler such as the NAG Fortran compiler;
- The NAG Fortran compiler also prints helpful error messages to help locate sources of bugs instead of the dreaded “segmentation fault”.

NAG Compiler Optional Argument Detection

- Compile command (if Forcheck cannot detect this):

```
nagfor -C=present arg_test.f90 -o arg_test.exe
```

- Fortran code:

```
call foo( a )
subroutine foo( a, b )
  real, intent(out) :: a
  real, intent(in), optional :: b
  a = b**2
end subroutine foo
```

- Helpful runtime error message and not just segmentation fault:

```
Runtime Error: arg_test.f90, line 14: Reference to OPTIONAL
argument B which is not PRESENT
```

NAG Compiler Dangling Pointer Detection

- Build command:

```
nagfor -C=dangling p_check.f90 -o p_check.exe
```

- Fortran code:

```
real, dimension(:), allocatable, target :: vec
real, dimension(:), pointer :: vec_p

allocate( vec(1:100) )
vec_p => vec
deallocate( vec )
print *, vec_p(:)
```

NAG Compiler Dangling Pointer Detection

- Runtime output - NAG compiler is the only Fortran compiler that can check this:

```
Runtime Error: p_check.f90, line 12: Reference to
dangling pointer VEC_P

Target was DEALLOCATEd at line 10 of
pointer_check.f90
```

NAG Compiler Undefined Variable Detection

- Compile command:

```
nagfor -C=undefined undef_test.f90 -o undef_test.exe
```

- Fortran code:

```
real, dimension(1:11) :: array
array(1:10) = 1.0
print *, array(1:11)
```

Runtime output:

```
Runtime Error: undef_test.f90, line 7: Reference to
undefined variable ARRAY(1:11)
Program terminated by fatal error
```

NAG Compiler Procedure Argument Detection

- Compile command:

```
nagfor -C=calls sub1.f90 -o sub1.exe
```

- Fortran code:

```
integer, parameter :: x = 12
call sub_test( x )
subroutine sub_test( x )
  integer :: x
  x = 10
end subroutine sub_test
```

- Runtime output:

```
Runtime Error: sub1.f90, line 13: Dummy argument X is
associated with an expression - cannot assign
```

NAG Compiler Integer Overflow Detection

- Compile command:

```
nagfor -C=intovf ovf_test.f90 -o ovf_test.exe
```

- Fortran code:

```
integer :: i, j, k

j = 12312312; k = 12312312
i = 12312312 * j * k
```

- Runtime output:

```
Runtime Error: ovf_test.f90, line 7: INTEGER(int32)
overflow for 12312312 * 12312312
Program terminated by fatal error
```

Conclusion

- More needs to be done to make code verification in computational science a mature practice just as it is in computer science;
- Develop a well-defined verification workflow and offer it as a service to the academic computational science community in the UK. *Verification as a service?*
- Promote verification tools and techniques;
- Just teaching a programming language is wholly insufficient. Code developers need much more support;
- Every community code should openly publish the results of their unit tests and tool verification results to quantify the quality of their code.