CCP5 Funding Application for the Fortran Modernisation Workshop

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1 Introduction

The Fortran Modernisation Workshop [7] is a two day event that was designed to address the software engineering needs specifically for the computational science community using the Fortran programming language. It covers the more modern features of Fortran, namely 90, 95, 2003 and 2008, to encourage attendees to modernise their legacy Fortran 77 and 66 codes. It also aims to teach attendees how to write portable, efficient, extensible and modular code in Fortran for multi-scale and multi-physics computational science. The workshop is run by a number of organisers which are listed in the author's list who are computational scientists with extensive coding experience, making them qualified to run this workshop. In addition, the Digital Technology Group from Cambridge University present their CamFort Fortran [4] verification tool and Allinea [1] present their debugging and profiling tools for Fortran at the workshop.

Although there are a number of Fortran and software engineering workshops run by the Archer HPC service and the Software Sustainability Institute, such workshops tend to be very generic and do not address any particular academic community which makes the Fortran Modernisation Workshop

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workshop very unique.

The topics that are covered in this workshop are listed below:

- Software engineering for computational science;
- Modern Fortran standards;
- NetCDF and HDF5 scientific file formats for data sharing in Fortran;
- GNU Automake to automate the build process;
- pFUnit unit testing framework for testing Fortran codes;
- Fortran verification using CamFort;
- Doxygen for Fortran code documentation;
- Git version control for collaborative code development;
- In-situ visualisation using PLplot in Fortran;
- IEEE floating point exception handling;
- Fortran interoperability with C, Python and R;
- Introduction to parallelism for Fortran;
- Debugging and profiling Fortran using Allinea DDT and MAP.

The technologies listed above cover the code development lifecycle as well as the computational science workflow, again making this workshop very unique and specific to computational science. Further information on the workflows can be found at [6]. The Fortran standards used by the attendees is shown in Figure 1.

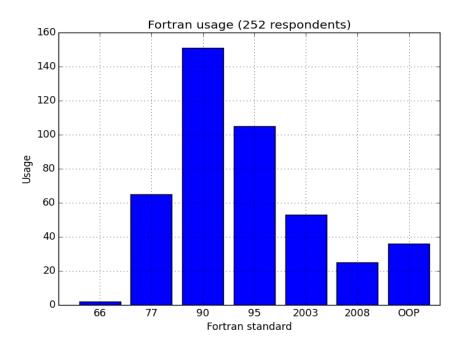


Figure 1: Fortran standards usage

Figure 1 shows that the most widely used standard is Fortran 90, but there still exists a number of Fortran 77 users. In addition, adoption of the newer standards such as 2003 and 2008 is still lacking which needs wider adoption that aids better software engineering. Thus, ones of the aims of the workshop is to address this shortfall.

The workshop feedback form listed the technologies that attendees intend to use which is shown in Figure 2 which shows that most attendees intend to use the modern features of Fortran.

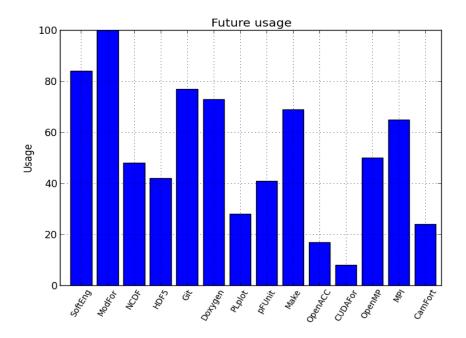


Figure 2: Future technology usage by attendees

What Figure 2 also shows that there is a lack of interest in Fortran verification techniques such as pFUnit and CamFort. This is a trend the workshop organisers have noticed and intend to emphasise the importance of code verification which is generally not very well covered for the Fortran programming language.

2 History of the Workshop

The Fortran Modernisation Workshop has been hosted at six sites which are listed in Table 1 with an average of 33.5 attendees per session. The workshop was rated by the attendees who gave it an average of 4.0 out of 5.

Site	Date	No. attendees	Rating
Cambridge University	March 2016	44	4.058/5
Oxford University	July 2016	31	3.52/5
University of Southampton	July 2016	44	4.286/5
CCFE	August 2016	11	3.445/5
Queen Mary London	September 2016	41	4.143/5
STFC Daresbury	October 2016	30	4.556/5

Table 1: Fortran Modernisation Workshop sessions

Blog posts on the Oxford University and University of Southampton workshops can be found at [5, 3]. The list of future workshop sessions are shown in Table 2 and the workshop organisers are in discussion with other sites regarding hosting the workshop.

Site	Date	Number of registrations
Manchester University	February 2017	22
University of Reading	February 2017	27

Table 2: Future Fortran Modernisation Workshop sessions

The registrations for the workshops listed in Table 2 are still open and are increasing.

3 Summary

As can be seen from Table 1 the workshop has been hosted at six sites and received very positive ratings. Future sessions are listed in Table 2 and the workshop is continuously being improved from the feedback received. The workshop was attended mainly by academics as well as attendees from industry, particularly at the STFC Daresbury session.

Computational chemistry codes are predominantly written in Fortran as well many other computational science codes in engineering and earth sciences. Fortran codes account for approximately 73% of CPU time on the Archer supercomputer [2], making Fortran the main programming language for computational science. For the compelling reasons outlined herein, we are requesting funding from CCP5 for the Fortran Modernisation Workshop. For further

questions, please feel free to contact me at fatima.chami@stfc.ac.uk or my colleagues fs395@cam.ac.uk or wadud.miah@nag.co.uk who will be happy to discuss this further.

References

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