

Proceedings

**International Workshop on
Software Engineering for Science
SE4Science 2016**

**16 May 2016
Austin, Texas, USA**

Proceedings

**International Workshop on
Software Engineering for Science
SE4Science 2016**

**16 May 2016
Austin, Texas, USA**



The Association for Computing Machinery
2 Penn Plaza, Suite 701
New York New York 10121-0701

ACM COPYRIGHT NOTICE. Copyright © 2016 by the Association for Computing Machinery, Inc. Permission to make digital or hard copies of part or all of this work for personal or classroom use is granted without fee provided that copies are not made or distributed for profit or commercial advantage and that copies bear this notice and the full citation on the first page. Copyrights for components of this work owned by others than ACM must be honored. Abstracting with credit is permitted. To copy otherwise, to republish, to post on servers, or to redistribute to lists, requires prior specific permission and/or a fee. Request permissions from Publications Dept., ACM, Inc., fax +1 (212) 869-0481, or permissions@acm.org.

For other copying of articles that carry a code at the bottom of the first or last page, copying is permitted provided that the per-copy fee indicated in the code is paid through the Copyright Clearance Center, 222 Rosewood Drive, Danvers, MA 01923, +1-978-750-8400, +1-978-750-4470 (fax).

Notice to Past Authors of ACM-Published Articles

ACM intends to create a complete electronic archive of all articles and/or other material previously published by ACM. If you have written a work that was previously published by ACM in any journal or conference proceedings prior to 1978, or any SIG Newsletter at any time, and you do NOT want this work to appear in the ACM Digital Library, please inform permissions@acm.org, stating the title of the work, the author(s), and where and when published.

ACM ISBN: 978-1-4503-4167-7

Editorial production by Patrick Kellenberger
Cover art production by Mark Bartosik



IEEE Computer Society
Conference Publishing Services (CPS)

<http://www.computer.org/cps>

Message from the Workshop Chairs

SE4Science 2016

Welcome to the 2016 International Workshop on Software Engineering for Science. The submissions covered a wide array of topics at the intersection of software engineering and scientific computing. This workshop contains two types of papers: *full papers (8 pages)* and *position papers (4 pages)*. After a thorough review and discussion process, the program committee and organizing committee accepted two full papers and four position papers for inclusion in the program.

The primary goal of this workshop is to facilitate the interaction among researchers from domains who do not usually have the opportunity to interact. As a result, this workshop always generates interesting and lively discussions. We expect that the papers accepted for this year's program will provide the necessary context and discussion points to once again have interesting and productive discussions. The organizing committee is committed to devoting a significant portion of the workshop time to small and large group discussions. Due to the large amount of time devoted to discussion, we encourage participation from interested researchers who do not have a paper on the program.

Organizer Carver would like to acknowledge partial support from NSF-1243887 and NSF-1445344. Organizer Chue Hong was supported by EPSRC Grant EP/H043160/1 and EPSRC/BBSRC/ESRC Grant EP/N006410/1.

Jeffrey C. Carver and Neil P. Chue Hong
SE4Science 2016 Co-Chairs

Committees

SE4Science 2016

Organizing Committee

Jeffrey C. Carver	University of Alabama, USA (Chair)
Neil P. Chue Hong	University of Edinburgh, UK (Co-Chair)

Program Committee

Ross Bartlett	Oak Ridge National Laboratory, USA
Michael Heroux	Sandia National Laboratories, USA
Lois McInnes	Argonne National Laboratory, USA
Marian Petre	Open University, UK
Damian Rouson	Sourcery, USA
George Thiruvathukal	Loyola University Chicago, USA

Sponsors and Supporters

ICSE 2016

Sponsors



Association for
Computing Machinery



Gold Benefactors



Silver Benefactors



Bronze Benefactors



IBM Research



Supporter



International Workshop on Software Engineering for Science (SE4Science 2016)

Table of Contents

Message from the Chairs	vi
Committees.....	vii
Sponsors and Supporters	viii

Paper Session 1

Nmag Micromagnetic Simulation Tool - Software Engineering Lessons Learned.....	1
<i>Hans Fangohr, Maximilian Albert, and Matteo Franchin</i>	
— <i>University of Southampton, United Kingdom of Great Britain and Northern Ireland</i>	
POSITION PAPER: Modularizing Global Variable In Climate Simulation Software	8
<i>Yuxing Ma, Tapajit Dey, and Audris Mockus</i>	
— <i>University of Tennessee-Knoxville, USA</i>	
POSITION PAPER: Documentation Generation from Annotated Source Code of Scientific Software.....	12
<i>Michael Moser and Josef Pichler</i>	
— <i>Software Competence Center Hagenberg GmbH, Austria</i>	

Paper Session 2

Experiences of Testing Bioinformatics Programs for Detecting Subtle Faults	16
<i>Anders Lundgren and Upulee Kanewala</i>	
— <i>Montana State University, USA</i>	
POSITION PAPER: A Knowledge-Based Approach to Scientific Software Development	23
<i>Dan Szymczak, Spencer Smith, and Jacques Carette</i>	
— <i>McMaster University, Canada</i>	
POSITION PAPER: An Evaluation Framework for Scientific Programming Productivity	27
<i>W.K Umayanganie Munipala and Shirley V. Moore</i>	
— <i>University of Texas at El Paso, USA</i>	

Author Index	31
--------------------	----