better scientific software

INTRODUCTION TO SOFTWARE TESTING FOR THE SCIENTIFIC COMMUNITY

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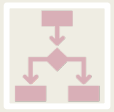
IOWA STATE UNIVERSITY OF SCIENCE AND TECHNOLOGY

Laboratory for Variability-Aware Assurance and Testing of Organic Programs LaVA-OPs

Module I: Overview

Motivation

What to test



Types of Testing

Models

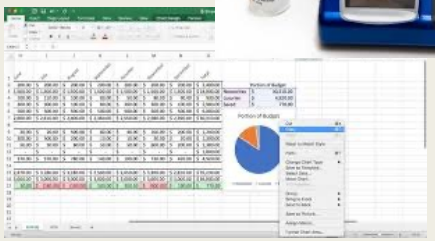
Coverage

Oracles

Software is Everywhere

Office

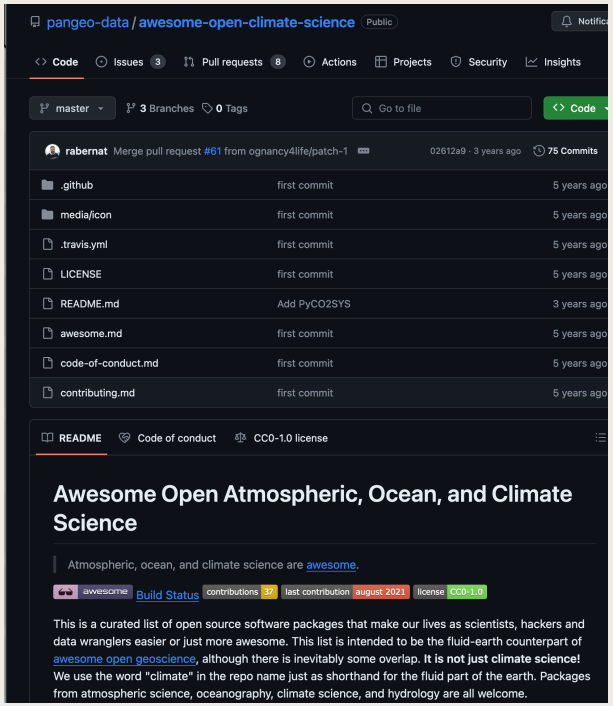
eclipse

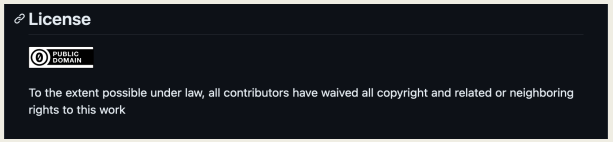


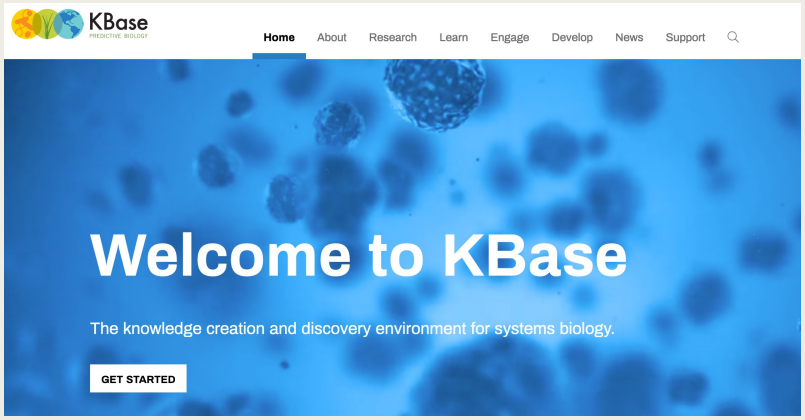
ABB

Linux

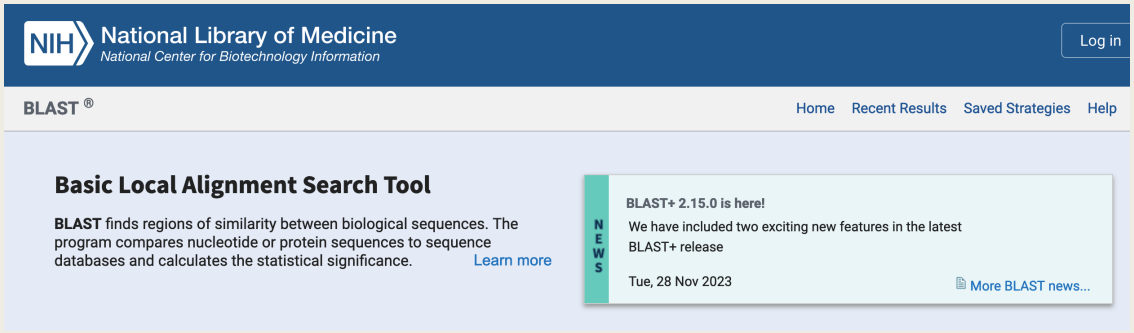
Software is Everywhere







Credit: DOE Systems Biology Knowledgebase



Credit: NCBI

When it Fails...

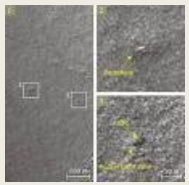
The Heartbleed Bug

The Heartbleed Bug is a serious vulnerability in the popular OpenSSL cryptographic software library. This weakness allows stealing the information protected, under normal conditions, by the SSL/TLS encryption used to secure the Internet. SSL/TLS provides communication security and privacy over the Internet for applications such as web, email, instant messaging (IM) and some virtual private networks (VPNs).

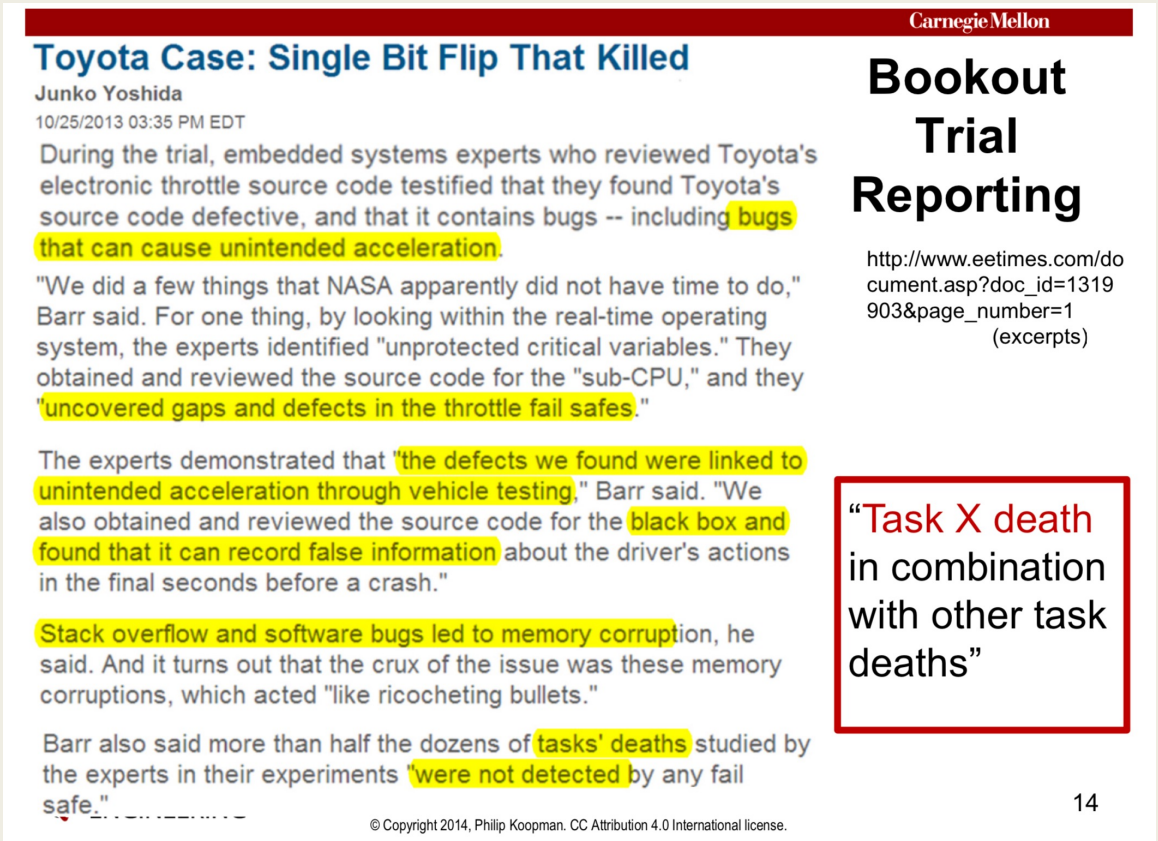
The Heartbleed bug allows anyone on the Internet to read th
the systems protected by the vulnerable versions of the Oper
software. This compromises the secret keys used to identify t
providers and to encrypt the traffic, the names and password
users and the actual content. This allows attackers to eavesdr
communications, steal data directly from the services and use
impersonate services and users.

- THERAC-25 radiation machine : Poor testing of safety-critical software can cost *lives* : 3 patients were killed

- NASA's Mars Lander: September 1999, crashed due to a units integration fault



Toyota Acceleration



Carnegie Mellon

Toyota Case: Single Bit Flip That Killed

Junko Yoshida

10/25/2013 03:35 PM EDT

During the trial, embedded systems experts who reviewed Toyota's electronic throttle source code testified that they found Toyota's source code defective, and that it contains bugs -- including bugs that can cause unintended acceleration.

"We did a few things that NASA apparently did not have time to do," Barr said. For one thing, by looking within the real-time operating system, the experts identified "unprotected critical variables." They obtained and reviewed the source code for the "sub-CPU," and they "uncovered gaps and defects in the throttle fail safes."

The experts demonstrated that "the defects we found were linked to unintended acceleration through vehicle testing," Barr said. "We also obtained and reviewed the source code for the black box and found that it can record false information about the driver's actions in the final seconds before a crash."

Stack overflow and software bugs led to memory corruption, he said. And it turns out that the crux of the issue was these memory corruptions, which acted "like ricocheting bullets."

Barr also said more than half the dozens of tasks' deaths studied by the experts in their experiments "were not detected by any fail safe."

Bookout Trial Reporting

http://www.eetimes.com/document.asp?doc_id=1319903&page_number=1 (excerpts)

"Task X death in combination with other task deaths"

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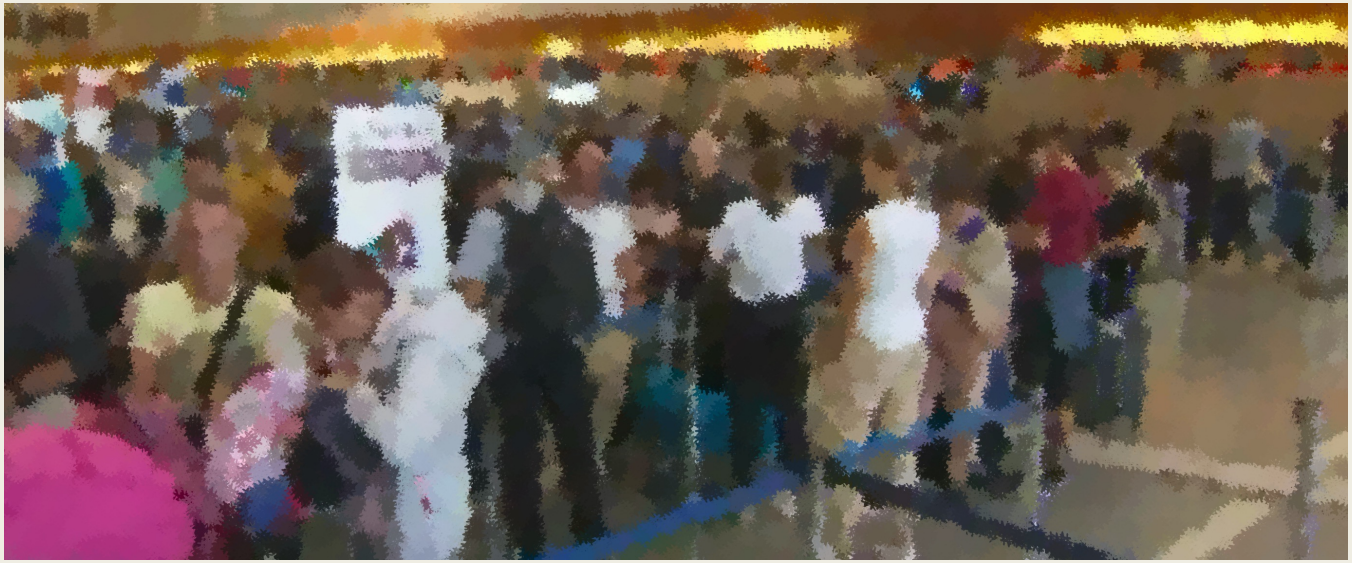
Aug 2019



- Customs processing at a big US International Airport, came to a stop

Consequences

- National Institutes of Standards (NIST)– up to $59 Billion per year – could be cut in ½ with better testing
- Government accountability report (GAO) report DOD loses $8 Billion annually due to rework [2004]

Consequences Cont.

- Huge losses due to web application failures
  - *Financial services : $6.5 million per hour (just in USA)*
  - *Credit card sales applications : $2.4 million per hour (in USA)*
  - *2007 : Symantec says that most security vulnerabilities are due to faulty software*

Why Scientific Software?

```
Error: NCBI C++ Exception:
T0 "/tmp/BLAST/2.11.0/gompi-2020b/ncbi-blast-2.11.0+-src/c++/src/serial/objistrasnb.cp
T0 "/tmp/BLAST/2.11.0/gompi-2020b/ncbi-blast-2.11.0+-src/c++/src/serial/member.cpp", l
```

Why Test Software?

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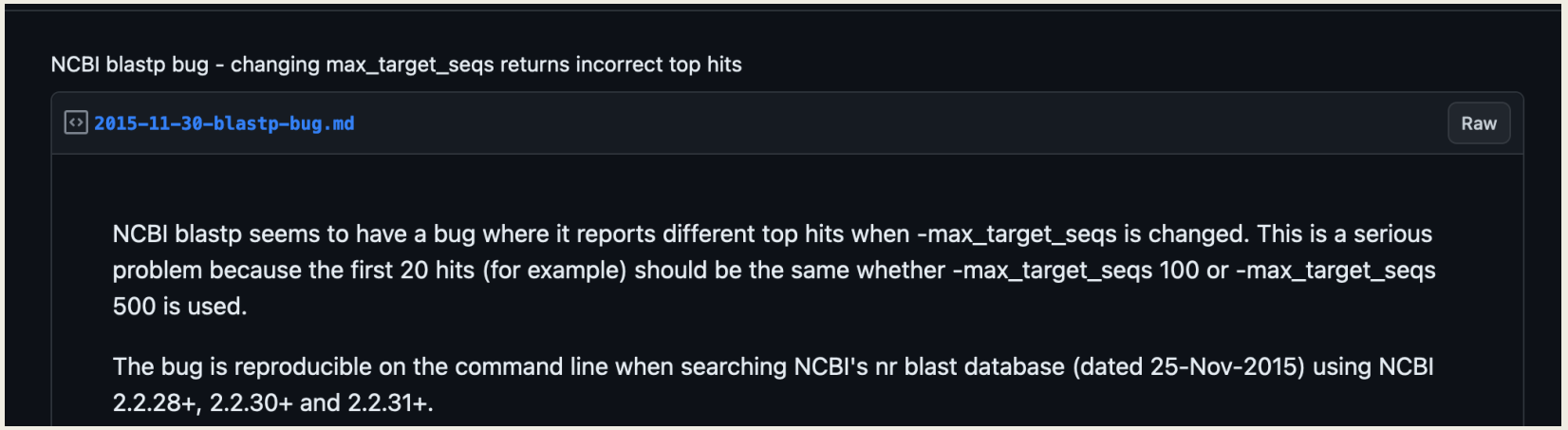
```

```
ial/objistrasnb.cpp", line 499: Error: (CSerialException::eOverflow) byte 132: overf
ial/member.cpp", line 767: Error: (CSerialException::eOverflow) ncbi::CMemberInfoFur
```

Why Test Software?



NCBI blastp bug - changing max_target_seqs returns incorrect top hits

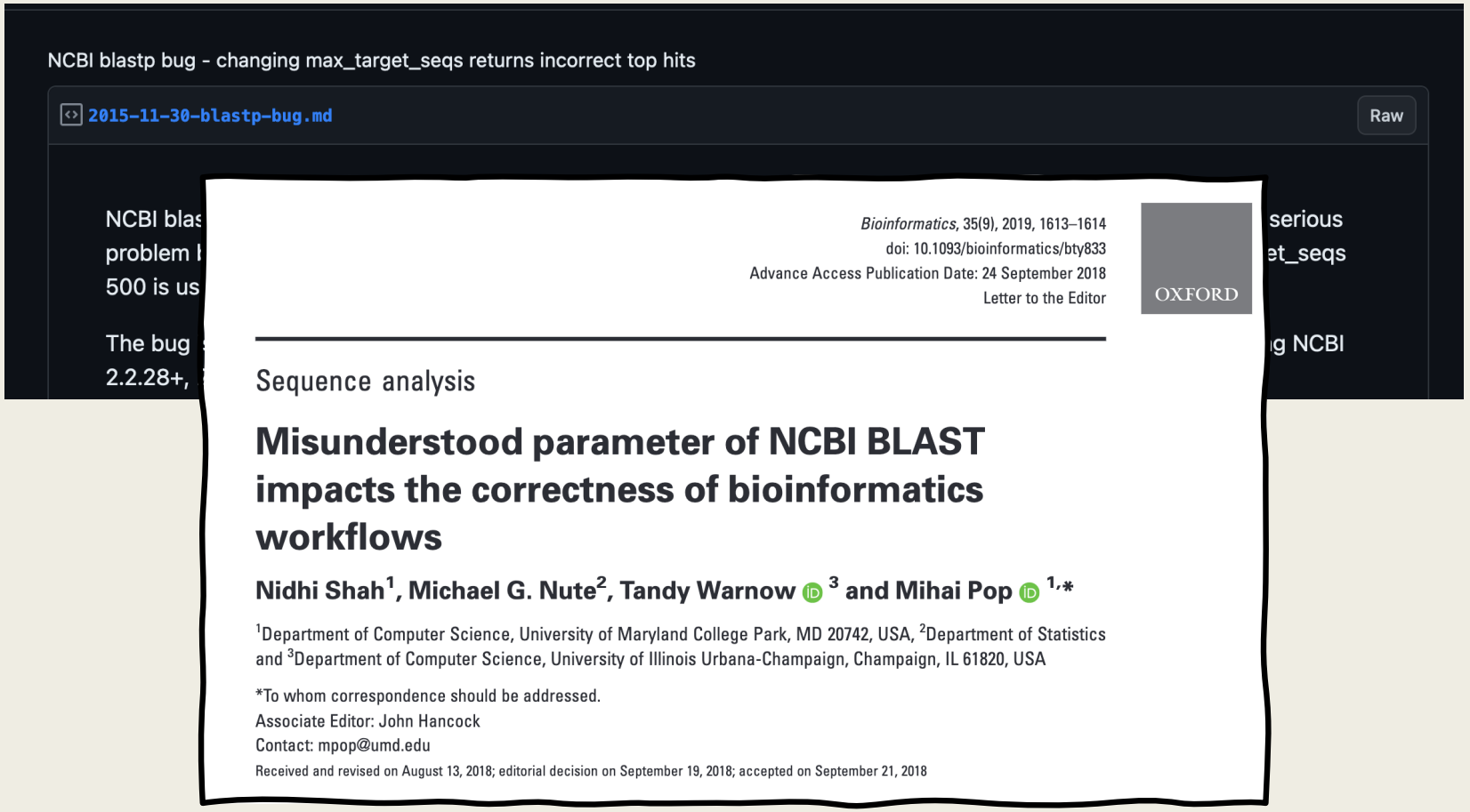
2015-11-30-blastp-bug.md

Raw

NCBI blastp seems to have a bug where it reports different top hits when -max_target_seqs is changed. This is a serious problem because the first 20 hits (for example) should be the same whether -max_target_seqs 100 or -max_target_seqs 500 is used.

The bug is reproducible on the command line when searching NCBI's nr blast database (dated 25-Nov-2015) using NCBI 2.2.28+, 2.2.30+ and 2.2.31+.

Why Test Software?



NCBI blastp bug - changing max_target_seqs returns incorrect top hits

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Raw

NCBI blas … serious
problem … et_seqs
500 is us …

The bug … g NCBI
2.2.28+, …

Bioinformatics, 35(9), 2019, 1613–1614
doi: 10.1093/bioinformatics/bty833
Advance Access Publication Date: 24 September 2018
Letter to the Editor

OXFORD

Sequence analysis

Misunderstood parameter of NCBI BLAST impacts the correctness of bioinformatics workflows

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Reply to the paper: Misunderstood parameters of NCBI BLAST impacts the correctness of bioinformatics workflows

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Why Test Software?

Dear Editor,

A recent letter by Shah *et al.* (2018) addressed the use of a command-line parameter in BLAST (Altschul *et al.*, 1997; Camacho *et al.*, 2009). BLAST is a very popular tool, so it is not surprising that this topic has provoked a great deal of interest. The authors have, however, conflated three different issues. One is a bug that will be fixed in the BLAST+ 2.8.1 release due out in December 2018, another is simply how BLAST works and the third might be viewed as a shortcoming of our implementation of composition-based statistics (CBS). Here, we address these issues and describe some new documentation about the BLAST process.

Shah et al. (2018) did not provide their own example in the letter, but later provided one at https://github.com/shahnidhi/BLAST_maxtargetseq_analysis. At the NCBI, we examined the new example and it became clear that the demonstrated behavior was a bug, resulting from an overly aggressive optimization, introduced in 2012 for BLASTN and MegaBLAST (DNA–DNA alignments). This bug has been fixed in the BLAST+ 2.8.1 release, due out in December 2018. The aberrant behavior seems to occur only in alignments with an extremely large number of gaps, which is the case in the example provided by Shah and collaborators.

Why Test Software?

contributed articles

DOI:10.1145/3382037

An approach to reproducibility problems related to porting software across machines and compilers.

BY DONG H. AHN, ALLISON H. BAKER, MICHAEL BENTLEY, IAN BRIGGS, GANESH GOPALAKRISHNAN, DORIT M. HAMMERLING, IGNACIO LAGUNA, GREGORY L. LEE, DANIEL J. MILROY, AND MARIANA VERTENSTEIN

Keeping Science on Keel When Software Moves

the machine instructions that actually get executed. Unfortunately, such changes do affect the computed results to a significant (and often worrisome) extent. In a majority of cases, there are not easily definable a priori answers one can check against. A programmer ends up comparing the new answer against a trusted baseline previously established or checks for indirect confirmations such as whether physical properties such as energy are conserved. However, such non-systematic efforts might miss underlying issues, and the code may keep misbehaving until these are fixed.

In this article, we present real-world evidence to show that ignoring numerical result changes can lead to misleading scientific conclusions. We present techniques and tools that can help computational scientists understand and analyze compiler effects on their scientific code. These techniques are applicable across a wide range of examples to narrow down the root-causes to single files, functions within files, and even computational expressions that affect specific variables. The developer may then rewrite the code selectively and/or suppress the application of certain optimizations to regain more predictable behavior.

Going forward, the frequency of required ports of computational software will increase, given that performance gains can no longer be obtained by mere-

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Why Test Software?

Merali, Zeeya. “Computational Science: ...Error.” *Nature* 467, no. 7317 (Oct, 2010): 775–77

Approaches to Avoid Failures

Static

Dynamic

Static Techniques

Analyze code without running the program

- Software inspections
  - *Analysis of source (and docs) against a checklist of common and historical defects*
- Software reviews
  - *Meetings of project personnel to discuss aspects of code/documents. May include stakeholders*

Static Techniques

Formal Verification

(1) Model checking

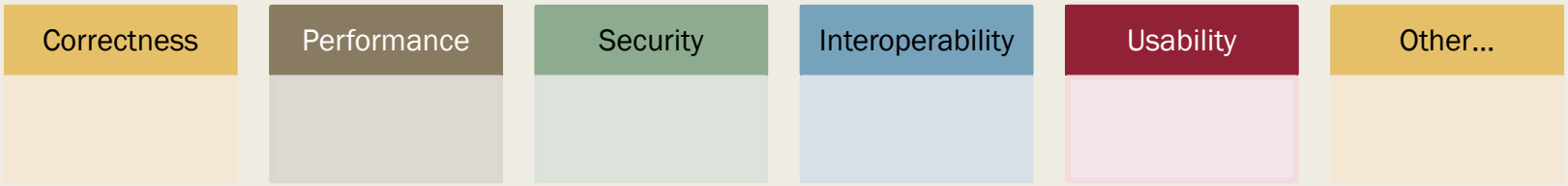
- Takes a model of the program (description of functional requirements) and properties that the program is supposed to satisfy
- Searches state-space to uncover violations of this property

(2) Theorem proving

Dynamic Technique

- Software Testing
  - *not complete* *(or exhaustive)*
  - *sound* *(if we find a fault it can happen)*

What Should We Test?



What Should We Test?

Correctness	Performance	Security	Interoperability	Usability	Other…
					• *Extensibility* • *Modularity*

What Should We Test?

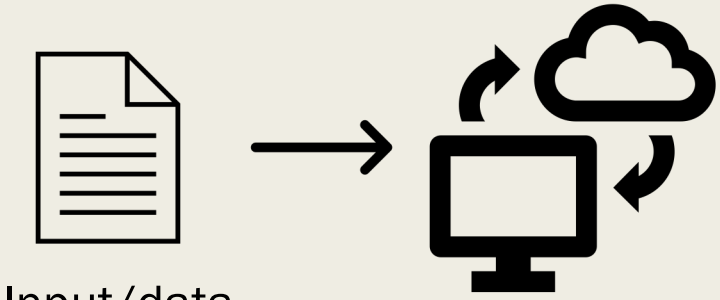
Correctness	Performance	Security	Interoperability	Usability	Other…
					• *Extensibility* • *Modularity*

Our focus will be on correctness and interoperability

What is Testing

Input/data

What is Testing



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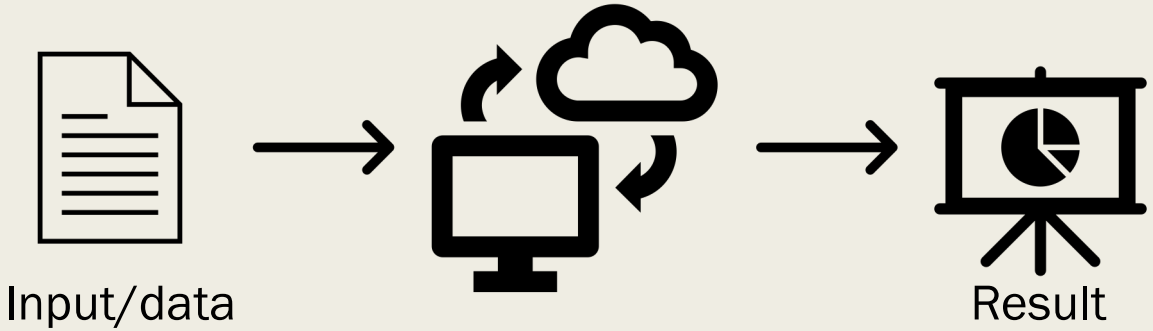

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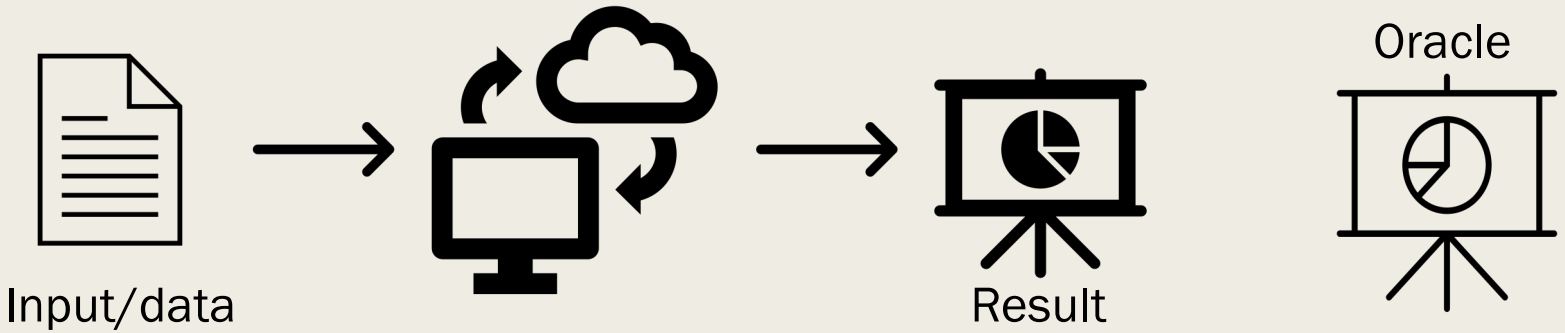

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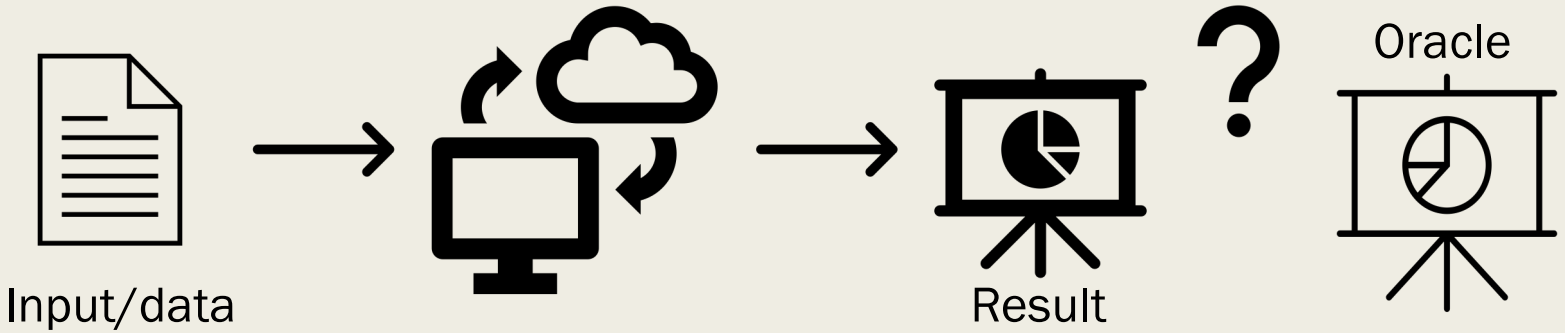
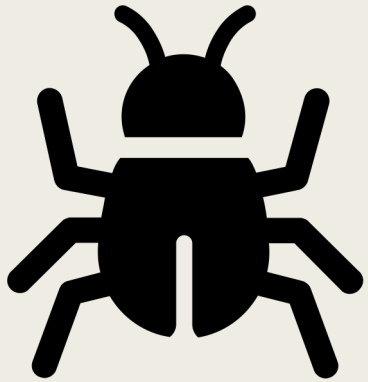


Limitations

Testing can only show the presence of faults.
It cannot determine their absence.

Edsger W. Dijkstra



Challenge

- To detect a program FAILURE we need to:
  - Reach a FAULT in the code
  - Infect the code (change to incorrect state) - ERROR
  - Propagate the error out of program
  - Reveal (detect) the error – (ORACLE)

RIPR model *Ammann, Offutt (Introduction to Software Testing, 2016)*

Tests Can Miss Faults

```python
def classify_triangle(a, b, c):
    # Sort the sides so that a <= b <= c
    if a > b:
        tmp = a
        a = tmp   #fault should be a=b
        b = tmp

    if a > c:
        tmp = a
        a = c
        c = tmp

    if b > c:
        tmp = b
        b = c
        c = tmp

    if a + b <= c:
        return TriangleType.INVALID
    elif a == b and b == c:
        return TriangleType.EQUILATERAL
    elif a == b or b == c:
        return TriangleType.ISOSCELES
    else:
        return TriangleType.SCALENE
```

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```

1. Test Case 3, 4, 5 (scalene)
   - doesn't reach fault

Tests Can Miss Faults

```python
def classify_triangle(a, b, c):
    # Sort the sides so that a <= b <= c
    if a > b:
        tmp = a
        a = tmp   #fault should be a=b
        b = tmp       5,5,1

    if a > c:
        tmp = a
        a = c
        c = tmp

    if b > c:
        tmp = b
        b = c
        c = tmp

    if a + b <= c:
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1. Test Case 3, 4, 5 (scalene)
   - doesn't reach fault

2. Test Case 5, 1, 1 (invalid)
   - reaches fault and infects
   - reveals (returns isosceles)

Tests Can Miss Faults

```python
def classify_triangle(a, b, c):
    # Sort the sides so that a <= b <= c
    if a > b:
        tmp = a
        a = tmp   #fault should be a=b
        b = tmp
    if a > c:
        tmp = a
        a = c
        c = tmp

    if b > c:
        tmp = b
        b = c
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    if a + b <= c:
        return TriangleType.INVALID
    elif a == b and b == c:
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    elif a == b or b == c:
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```

2,2,-1

1. Test Case 3, 4, 5 (scalene)
   - doesn't reach fault

2. Test Case 5, 1, 1 (invalid)
   - reaches fault and infects
   - reveals (returns isosceles)

3. Test Case 2, 1, -1 (invalid)
   - reaches fault and infects
   - Doesn't propagate (2, 2,-1) is still INVALID

Software vs. Data

Scientific software is often data (or model driven)

Both software and data can lead to faults

We start by focusing on software

But I Have Unit Tests…

These are an essential part of testing

Focus is on individual modules

Can be re-used each time system changes (regression testing)

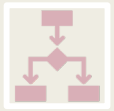
Can be packaged with software when released

Other testing focuses on the system specifications and overall program behavior

Module I: Overview


Motivation


What to test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