Improving Scientific Software Quality

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- Why do we need to talk about software quality?
- What is software quality?
- How can test driven development improve software quality?

Why do we need to talk about it?

“Existing models are known to have high levels of software quality”

(B. N. Lawrence et al, Crossing the Chasm: how to develop weather and climate models for next generation computers?, 2018)

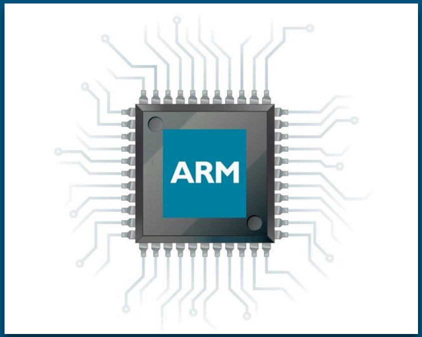
Why do we need to talk about it?

“The [nuclear engineering code], in spite of the aspirations of its designers, amounted to no more than a very expensive random number generator”

(L. Hatton, The T Experiments: Errors in scientific software, 1997)

Why do we need to talk about it?

- Poor quality has far reaching consequences
- Wide range of scientific software development practices
- Software quality throttles scientific progress
- Time to develop a new model is longer than the lifespan of the new hardware



What is it?


Scientific Software
do j=2,ny-1
do i=2,nx-1
u_new(i,j) = ((u(i+1,j) + u(i-1,j) + u(i,j+1)
- 0.5_r8kind * dtdx * ((u(i+1,j)**2
- 0.5_r8kind * dtdy * (v(i,j)) *
- 0.5_r8kind * g * dtdx * (h(i+1,j)
Quality

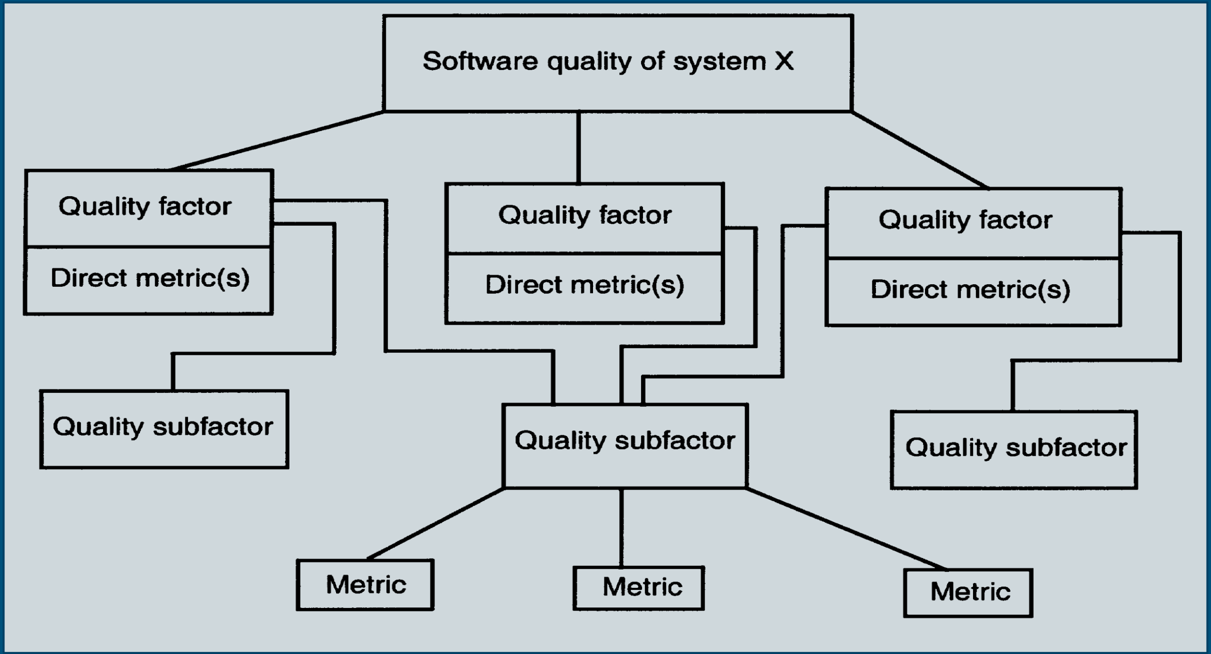
What is it?

- The bad news
  - There is no objective definition of software quality
  - Can’t be measured accurately/easily
  - Hard to prove that software engineering practices determine quality

What is it?

- The bad news
  - There is no objective definition of software quality
  - Can't be measured accurately/easily
  - Hard to prove that software engineering practices determine quality
- The good news
  - There are some good ideas and standards
  - Some things are quantifiable
  - Studies show rigorous testing decreases defect density

What is it?



IEEE Std 1061™-1998 (R2009) - A Software Quality Metrics Methodology

What is it?

- Functional Suitability
- Usability
- Reliability
- Maintainability
- Performance Efficiency
- Compatibility
- Security
- Portability

ISO/IEC 25010:2011 Software Quality Model Standard Attributes

What is it?

Functional Suitability	Usability	Reliability	Maintainability
Performance Efficiency	Compatibility	Security	Portability

Scientific Software Quality Attribute Priorities

What is it?

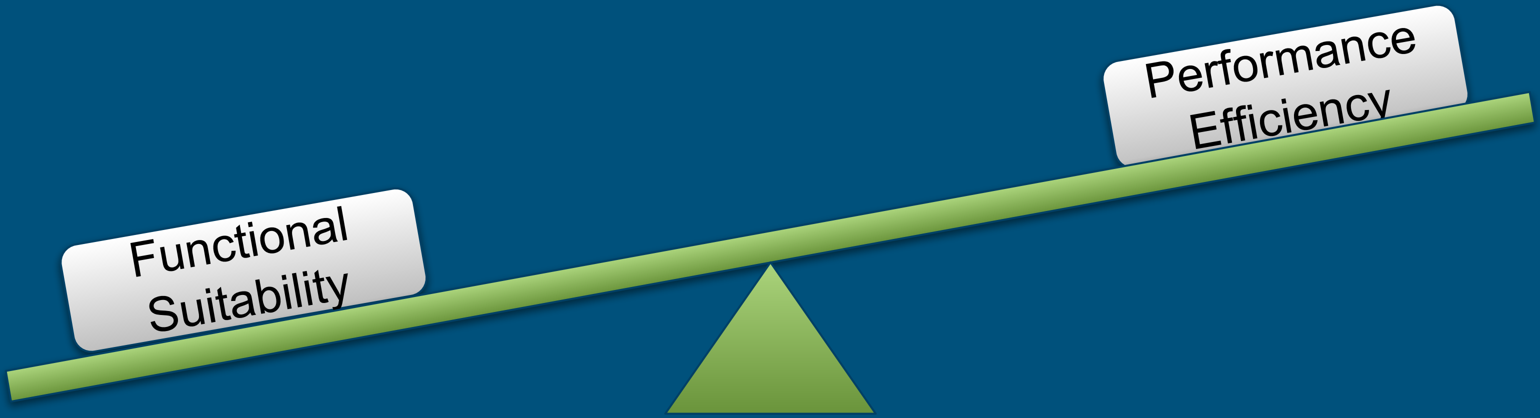
No one knows I exist...

Why does everyone ignore me?

Functional Suitability	Usability	Reliability	Maintainability
Performance Efficiency	Compatibility	Security	Portability

Scientific Software Quality Attribute Priorities

What is it?



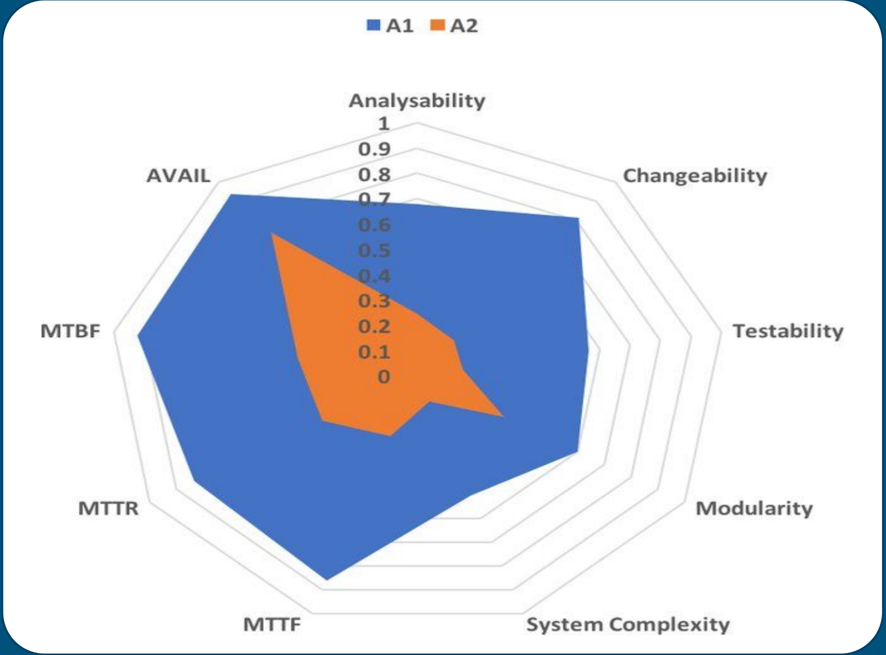
Perceived Scientific Software Quality Tradeoffs

What is it?

Perceived Scientific Software Quality Tradeoffs

What is it?

- Scientific software quality models do exist
- Does/should anyone use them?
- Metrics for quality components
  - Complexity → Maintainability
  - Defect density → Reliability
- Some scientific quality models lack important attributes



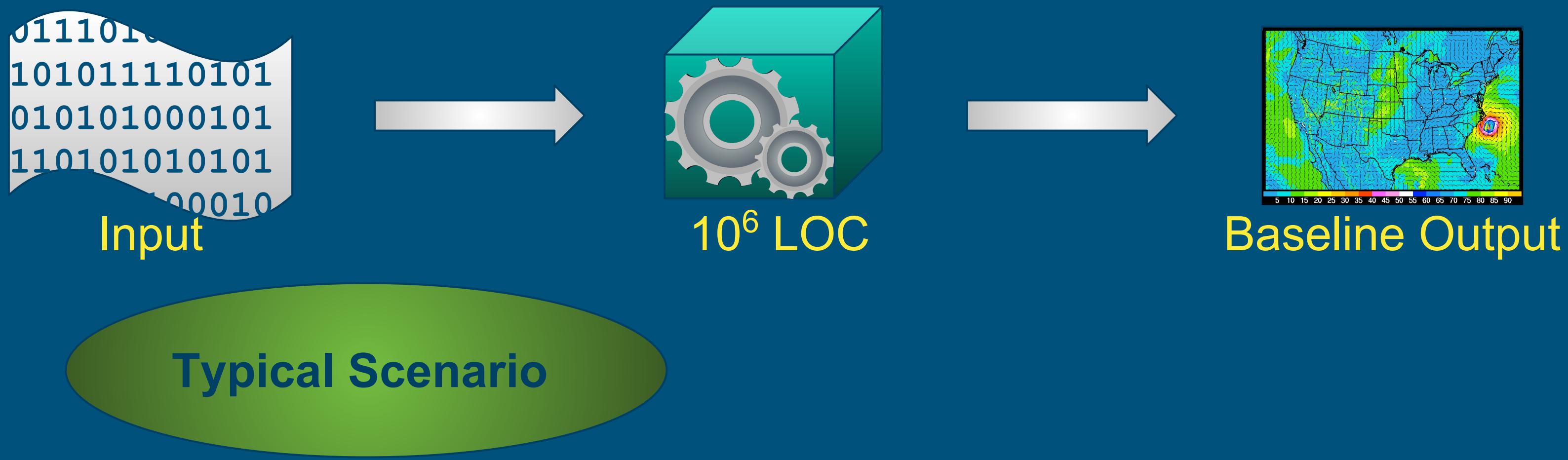
(B. Koteska, A. Mishev, L. Pejov, Quantitative Measurement of Scientific Software Quality: Definition of a Novel Quality Model, March 2018)

What is it?

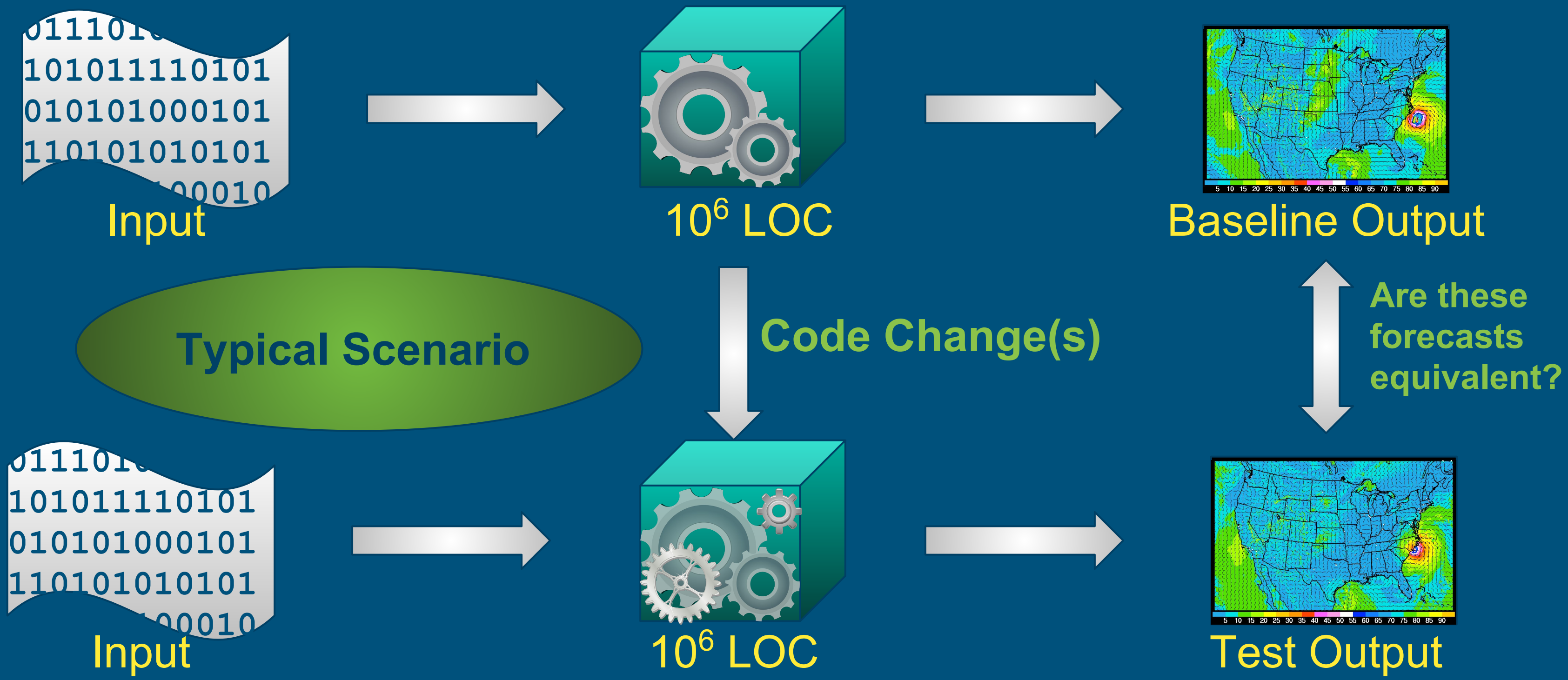
Challenges Specific to Scientific Software

- Capacity for scientific insight is an important quality attribute
- “Scientific software quality” conflates science and software
  - Theoretical system, computational system, software implementation
- Requirements are often poorly defined up front
- Requirements driven by scientific discovery process
- Evolving requirements make extensibility and reproducibility difficult
- Oracle & tolerance problems make correctness difficult to measure

How Can Test Driven Development Help?



How Can Test Driven Development Help?



How Can Test Driven Development Help?

Several problems with reliance on system level tests

- Focus is on testing the “model” instead of the “software”
- Does not provide error localization when failures are detected
- Trillions of operations performed exacerbate comparison of results
- High levels of test coverage are difficult to achieve
- Often masks serious errors
- Undetected bugs are allowed into the “stable” repository branches

How Can Test Driven Development Help?

A better way....

- Test the science AND the software
  - Theoretical system, computational system, software implementation
- Test multiple quality factors
  - Performance, reliability, correctness, portability
- Test at all granularities
  - Unit tests, integration tests, system tests
- Write new code → Write new tests

How Can Test Driven Development Help?

Rules of engagement

- Automate tests / continuous integration
- Require pull requests for all merges
- Require reviews for all pull requests
- No pull requests are merged unless all tests pass
- Pull requests must supply tests for all new code

```
Test project /scratch4/BMC/gsd-hpcs/Christopher.W.Harrop/Exascale-DA/build_theia_intel
      Start  1: shallow_water_config_arglist
 1/16 Test  #1: shallow_water_config_arglist ...........   Passed    0.01 sec
      Start  2: shallow_water_config_nlfile
 2/16 Test  #2: shallow_water_config_nlfile ............   Passed    0.01 sec
      Start  3: shallow_water_config_nlunit
 3/16 Test  #3: shallow_water_config_nlunit ............   Passed    0.01 sec
      Start  4: shallow_water_model_matlab_regression
 4/16 Test  #4: shallow_water_model_matlab_regression ...   Passed   22.94 sec
      Start  5: shallow_water_model_init_default
 5/16 Test  #5: shallow_water_model_init_default ........   Passed    0.01 sec
      Start  6: shallow_water_model_init_optional
 6/16 Test  #6: shallow_water_model_init_optional .......   Passed    0.01 sec
      Start  7: shallow_water_model_adv_nsteps
 7/16 Test  #7: shallow_water_model_adv_nsteps .........   Passed    0.01 sec
      Start  8: shallow_water_model_regression
 8/16 Test  #8: shallow_water_model_regression .........   Passed    0.02 sec
      Start  9: shallow_water_reader
 9/16 Test  #9: shallow_water_reader ...................   Passed    0.01 sec
      Start 10: shallow_water_writer
10/16 Test #10: shallow_water_writer ...................   Passed    0.02 sec
      Start 11: shallow_water_tl_init_default
11/16 Test #11: shallow_water_tl_init_default ..........   Passed    0.01 sec
      Start 12: shallow_water_tl_init_optional
12/16 Test #12: shallow_water_tl_init_optional .........   Passed    0.01 sec
      Start 13: shallow_water_tl_adv_nsteps
13/16 Test #13: shallow_water_tl_adv_nsteps ............   Passed    0.19 sec
      Start 14: shallow_water_adj_init_default
14/16 Test #14: shallow_water_adj_init_default .........   Passed    0.01 sec
      Start 15: shallow_water_adj_init_optional
15/16 Test #15: shallow_water_adj_init_optional ........   Passed    0.01 sec
      Start 16: shallow_water_adj_adv_nsteps
16/16 Test #16: shallow_water_adj_adv_nsteps ...........   Passed    0.20 sec

100% tests passed, 0 tests failed out of 16

Total Test time (real) =  23.55 sec
[Christopher.W.Harrop@Theia:tfe03 build_theia_intel]$
```

Conclusions

- We can learn from commercial software engineering industry
- Maintainability should be prioritized
- Test-driven development should be adopted to reduce defect density
- Test automation should be maximized to minimize human error

Backup Slides

What is it?

ISO/IEC 25010:2011 Quality Model

Functional Suitability

- Functional Completeness
- Functional Correctness
- Functional Appropriateness

What is it?

ISO/IEC 25010:2011 Quality Model

Performance Efficiency

- Time Behavior
- Resource Utilization
- Capacity

What is it?

ISO/IEC 25010:2011 Quality Model

Compatibility

- Co-existence
- Interoperability

What is it?

ISO/IEC 25010:2011 Quality Model

Usability

- Appropriateness Recognizability
- Learnability
- Operability
- User Error Protection
- User Interface Aesthetics
- Accessibility

What is it?

ISO/IEC 25010:2011 Quality Model

Reliability

- Maturity
- Availability
- Fault Tolerance
- Recoverability

What is it?

ISO/IEC 25010:2011 Quality Model

Security

- Confidentiality
- Integrity
- Non-repudiation
- Authenticity
- Accountability

What is it?

ISO/IEC 25010:2011 Quality Model

Maintainability

- Modularity
- Reusability
- Analysability
- Modifiability
- Testability

What is it?

ISO/IEC 25010:2011 Quality Model

Portability

- Adaptability
- Installability
- Replaceability

What is it?

IEEE Std 1061™-1998 (R2009) - A Software Quality Metrics Methodology

- Goals
  - Assess achievement of quality goals;
  - Establish quality requirements for a system at its outset;
  - Establish acceptance criteria and standards;
  - Evaluate the level of quality achieved against the established requirements;
  - Detect anomalies or point to potential problems in the system;
  - Predict the level of quality that will be achieved in the future;
  - Monitor changes in quality when software is modified;
  - Assess the ease of change to the system during product evolution;
  - Validate a metrics set