Test Driven Development of Scientific Models

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Outline

1. Motivations
2. Testing
3. Testing Frameworks
4. Test-driven Develompent (TDD)
5. What about numerical software?

Motivation 1: Fear/Stress

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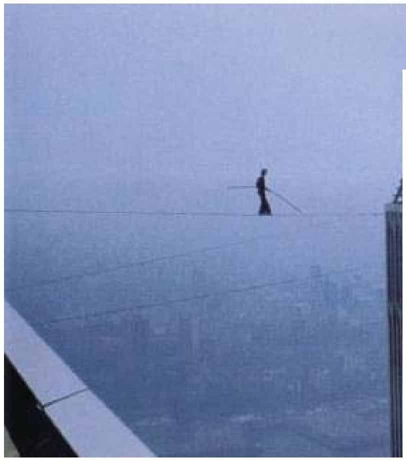

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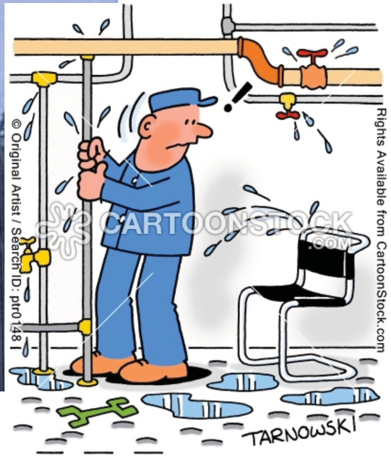
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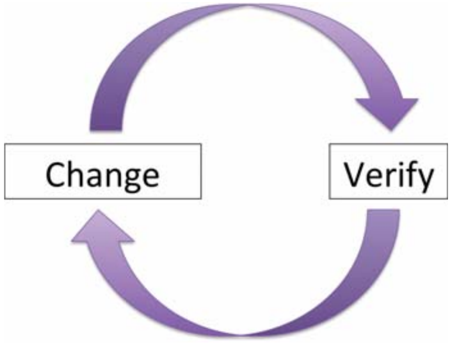
Motivation 1: Fear/Stress

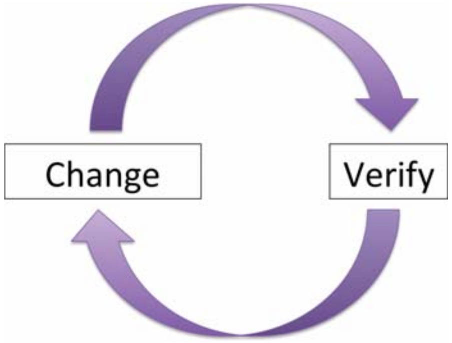
Calvin & Hobbes - Bill Waterson

Motivation 2: Productivity



Motivation 2: Productivity

- **New feature**
- **Refactor**



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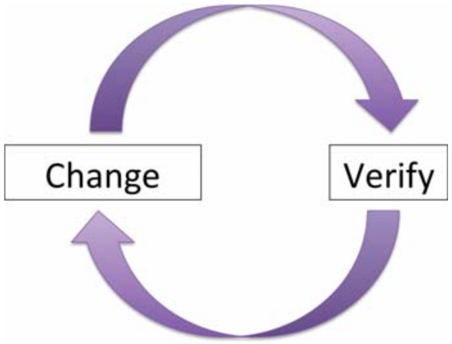

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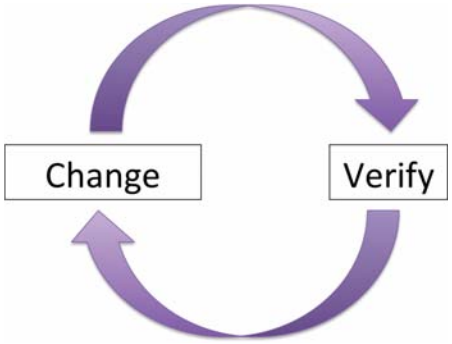

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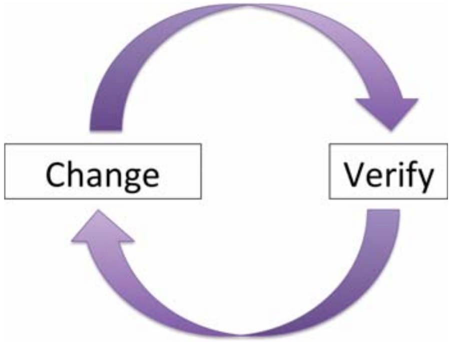

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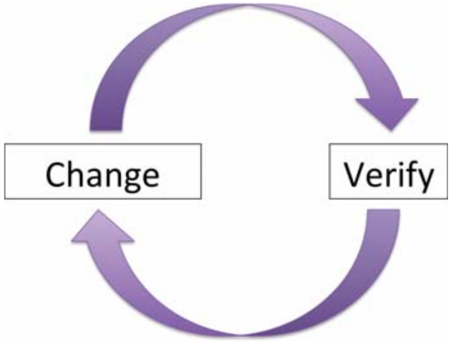

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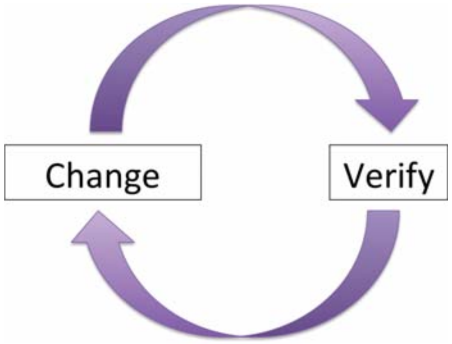

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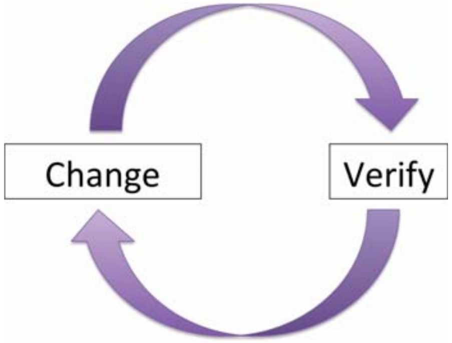

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What is the latency of verification for large scientific models?

Some observations about human behavior:

- Risk of defects scales with magnitude of change per iteration
- Development time per iteration will be comparable to verification time

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Conclusion:
Productivity is a nonlinear function of the cost of verification!

Motivation 3: The Limelight

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    - ★ Those which change results below detection threshold

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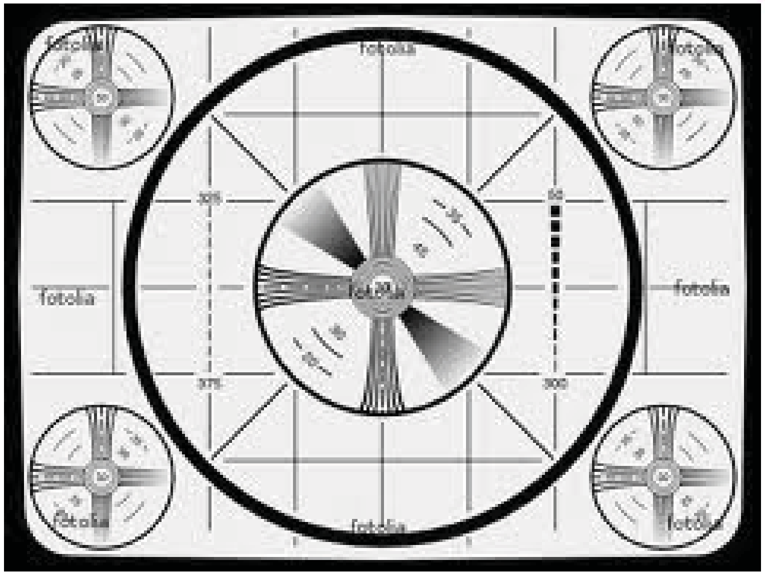
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Test Harness - work in safety

Collection of tests that constrain system

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- **Inexpensive compared to application (ideally)**

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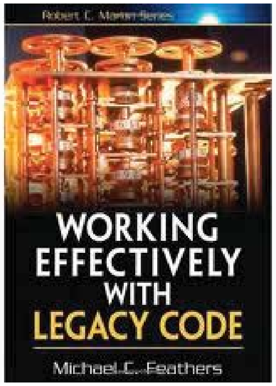
Michael Feathers
Working Effectively with Legacy Code



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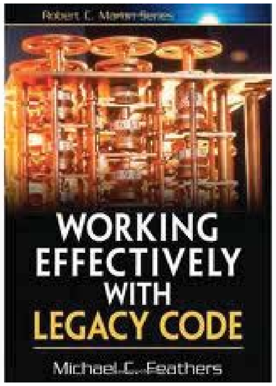

"Fear is the path to the dark side. Fear leads to anger. Anger leads to hate. Hate leads to suffering." - Yoda

starwars.wikia.com

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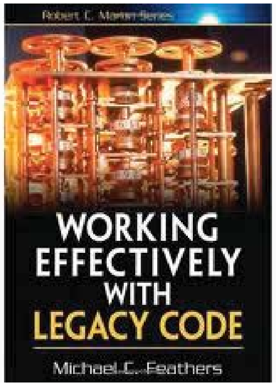

- Lack of tests leads to fear of introducing subtle bugs and/or changing things inadvertently.
- Also is a barrier to involving pure software engineers in the development of our models.

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  http://java.dzone.com/articles/unit-test-excuses
  - James Sugrue

- **Numeric/scientific code cannot be tested, because ...**

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- Clear intent

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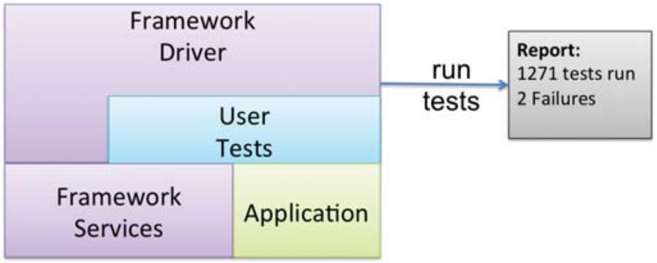
Testing Frameworks



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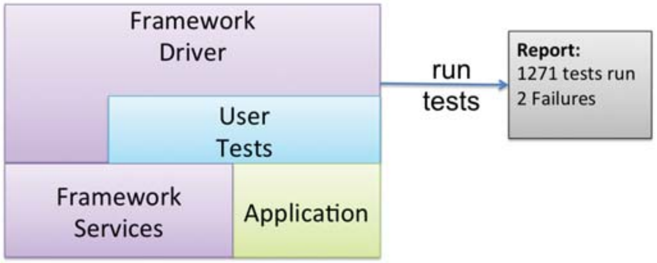

- Key services
  - Provide methods to succinctly express expected values

    ```
    call assertEqual(120, factorial(5))
    ```

  - Register test procedures with framework
  - Execute test procedures, and summarize success/failure

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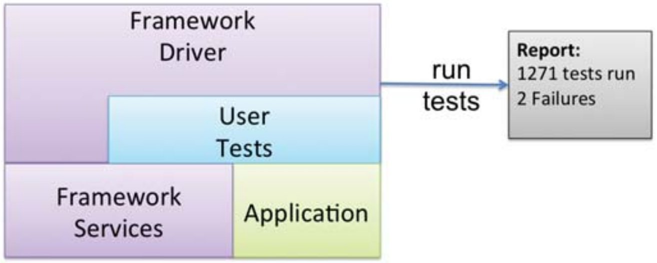

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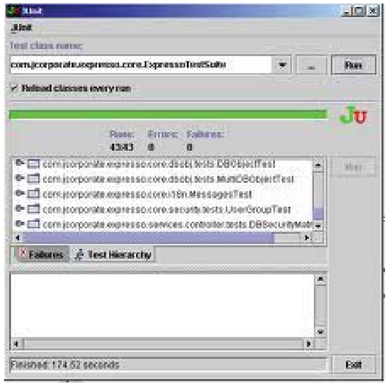
  - Register test procedures with framework
  - Execute test procedures, and summarize success/failure
- Generally specific/customized to programming language (xUnit)
  - Java (JUnit)
  - Python (pyUnit)
  - C++ (cxxUnit, cppUnit)
  - Fortran (FRUIT, FUNIT, **pFUnit**)

Frameworks and IDE's

Frameworks are often integrated within IDEs for even greater ease of use:



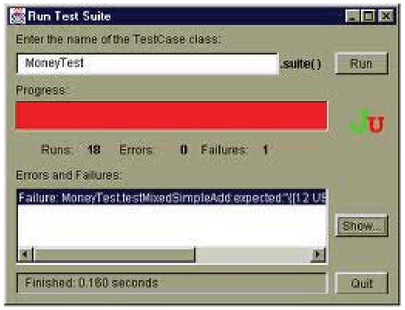
Test class name: com.jcorporate.expresso.core.ExpressoTestSuite

✓ Reload classes every run

Runs: 43/43 Errors: 0 Failures: 0

```
com.jcorporate.expresso.core.dbobj.tests.DBObjectTest
com.jcorporate.expresso.core.dbobj.tests.MultiDBObjectTest
com.jcorporate.expresso.core.i18n.MessagesTest
com.jcorporate.expresso.core.security.tests.UserGroupTest
com.jcorporate.expresso.services.controller.tests.DBSecurityMatr
```

Finished: 174.52 seconds



Enter the name of the TestCase class: MoneyTest .suite()

Progress:

Runs: 18 Errors: 0 Failures: 1

Errors and Failures:

```
Failure: MoneyTest.testMixedSimpleAdd:expected:"{[12 US
```

Finished: 0.160 seconds

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Today I am here to sell you something ...

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- Tests written by separate team (black box testing)
- Tests written *after* implementation

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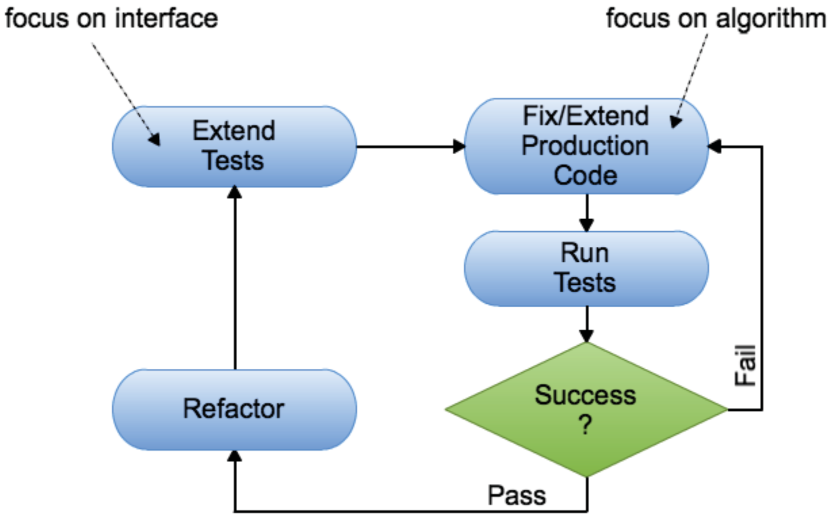
New paradigm - Test-driven development (TDD)

- Developers write the tests (white box testing)
- Tests written *before* production code
- *Enabled by emergence of strong unit testing frameworks*

The TDD cycle



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- **High quality implementation?**
    - Emphasis on interfaces
    - Testable code is cleaner code.

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- Lack of known (nontrivial) solutions
- Irreducible complexity?
- Stability - issues that occur after long integrations
- Emergent properties of coupled systems (including stability)

Numerical error

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Unfortunately ...

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- Best case scenario is usually some asymtotic form with unknown leading coefficient!

TDD techniques in presence of numerical error

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    - Often more appropriate as *validation* test
2. Nonlinearity - use tailored synthetic inputs:
    - E.g., choose values to make denominators O(1)
3. Composition/iteration: test steps in isolation:
    - Allows choice of tailored synthetic inputs at *each* step
    - Test iteration *logic* not *accumulation*

Example - testing layers in isolation

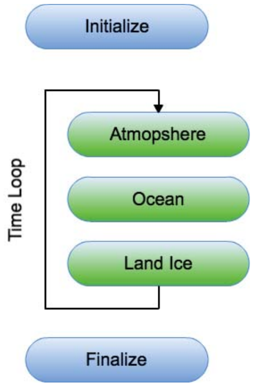
Consider the main loop of a climate model:

Do test

- Proper # of iterations
- Pieces called in correct order
- Passing of data between components

Do NOT test

- Calculations inside components



Easier with *objects* than with procedures.

TDD without “known” solutions

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But still use high level analytic solutions as tests when available!

TDD and irreducible complexity

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  - Unit tests use tailored inputs
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  - Models *couple* many components/algorithms ⇒ exponential complexity
  - Tests are *decoupled* ⇒ linear complexity

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  4. Insufficient physical fidelity - science issue (testing is not magic)
- At the very least, TDD can reduce the frequency with which one must perform long integrations

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- TDD emphasizes small fine-grained implementations
- Such implementations are often sub-optimal in terms of performance
- Optimized implementations typically fuse multiple operations
- Solution: bootstrapping
  - Use initial TDD solution as unit test for optimized implementation
  - Maintain *both* implementations (and tests)

TDD and the burden of legacy code

- TDD was created for developing *new* code, and does not directly speak to testing legacy code.
- Best practice for incorporating new functionality:
  - Avoid *wedging* new loging directly into existing large procedure
  - Use TDD to develop separate facility for new computation
  - Just *call* the new procedure from the large legacy procedure
- Refactoring
  - Use unit tests to constrain existing behavior
  - Very difficult for large procedures
  - Try to find small pieces to pull out into new procedures

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Summary

- TDD can be applied to scientific models
- Tool support exists (unabashed plug for pFUnit tutorial)
- Cost/benefit analysis for numerical software needs further study

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Test-Driven Development: By Example - Kent Beck