Test Driven Development of Scientific Models
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Outline

1 Motivations

2 Testing

3 Testing Frameworks

4 Test-driven Development (TDD)

5 What about numerical software?
Motivation 1: Fear/Stress
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[Image with a cartoon of a person working on pipes, labeled 'NASA.']

photomatt7.wordpress.com

www.cartoonstock.com
Motivation 1: Fear/Stress

Calvin & Hobbes - Bill Waterson
Motivation 2: Productivity
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- New feature
- Refactor

Change  
Verify
Motivation 2: Productivity
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Compiles?
Executes?

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- Really correct?
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Motivation 2: Productivity

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

Climate modeling has grown to be of extreme socioeconomic importance:

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- Adaptation/mitigation strategies easily exceed $100 trillion\(^1\)

\(^1\)Pearce, Fred. “Top economist counts future cost of climate change.”
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  - Those which change results below detection threshold

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Test Harness - work in safety

Collection of tests that constrain system
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- Inexpensive compared to application (ideally)
Do you write legacy code?
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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
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*Working Effectively with Legacy Code*

- 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.
Excuses, excuses ...
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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

- 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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    ```java
call assertEqual(120, factorial(5))
    ```
  - 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:
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Today I am here to sell you something ...
Old paradigm:

- Tests written by separate team (black box testing)
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Consequences:
- Testing schedule compressed for release
- Defects detected late in development ($$)
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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

- Extend Tests
  - Focus on interface
- Fix/Extend Production Code
- Run Tests
- Success? (Decision)
- Fail
- Pass
- Refactor
  - Focus on algorithm
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- **High quality implementation?**
  - Emphasis on interfaces
  - Testable code is cleaner code.
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Unique testing challenges of numerical software
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- Stability - issues that occur after long integrations
- Emergent properties of coupled systems (including stability)
Numerical error

Testing numerical algorithms requires an *accurate* estimate for tolerance:
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Unfortunately ...
- Error estimates are seldom available for complex algorithms
- Best case scenario is usually some asymptotic form with unknown leading coefficient!
TDD techniques in presence of numerical error
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Sources:
TDD techniques in presence of numerical error

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1. Approximation
TDD techniques in presence of numerical error

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TDD techniques in presence of numerical error

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Mitigation strategies:
TDD techniques in presence of numerical error

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Mitigation strategies:
- Approximation:
  - Test the implementation not the math (i.e., duck)
  - Often more appropriate as validation test
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Mitigation strategies:

- Approximation:
  - Test the *implementation* not the *math* (i.e., duck)
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- Nonlinearity - use tailored synthetic inputs:
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Mitigation strategies:
1. Approximation:
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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

Consider the apparent contradiction:
TDD without "known" solutions

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- Complex algorithms yield few nontrivial analytic solutions.
- Implementations are not random keystrokes
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- Apparently analytic solutions are unnecessary!
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**Tests should only verify translation, not validity of algorithms**

- Test each step in isolation
- Tailor synthetic inputs to yield “obvious” results for each step
- Separately test that steps are composed correctly
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*But still use high level analytic solutions as tests when available!*
TDD and irreducible complexity

“Aren’t my tests as complex as the implementation?”
“Aren’t my tests just repeating logic in the implementation?”
TDD and irreducible complexity

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  - Models *couple* many components/algorithms ⇒ exponential complexity
  - Tests are *decoupled* ⇒ linear complexity
TDD and emergent properties

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- At the very least, TDD can reduce the frequency with which one must perform long integrations
TDD and performance

- TDD emphasizes small fine-grained implementations
- Such implementations are often sub-optimal in terms of performance
- Optimized implementations typically fuse multiple operations
TDD and performance

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- 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 logging 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
Acknowledgements

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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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http://pfunit.sourceforge.net
Test-Driven Development: By Example - Kent Beck