Test Driven Development of Scientific Models

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Tom Clune

Advanced Software Technology Group
Computational and Information Sciences and Technology Office
NASA Goddard Space Flight Center
Outline

1 Motivations

2 Testing

3 Testing Frameworks

4 Test-driven Development (TDD)

5 What about numerical software?
Motivation 1: Fear/Stress
Motivation 1: Fear/Stress

photomatt7.wordpress.com
Motivation 1: Fear/Stress
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Motivation 2: Productivity
Motivation 2: Productivity

- New feature
- Refactor

Change  Verify
Motivation 2: Productivity

- New feature
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- Compiles?
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- 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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- Validation cannot detect certain types of software defects:

\(^1\)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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- Too difficult to maintain tests
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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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  - No STDOUT; temp files deleted; ...
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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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    ```python
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)

Report: 1271 tests run 2 Failures
Frameworks and IDE's

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

1. Motivations
2. Testing
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4. Test-driven Development (TDD)
5. What about numerical software?
Today I am here to sell you something ...
Old paradigm:
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- Tests written after implementation
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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**
- **Fix/Extend Production Code**
- **Run Tests**
- **Refactor**

**Success**

- Focus on interface
- Focus on algorithm

**Pass**

**Fail**
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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

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Unfortunately ...
- Error estimates are seldom available for complex algorithms
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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

Sources:
- Approximation
- Nonlinearity - e.g., small denominators
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:
1. Approximation:
   - Test the implementation not the math (i.e., duck)
   - Often more appropriate as validation test
TDD techniques in presence of numerical error

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Mitigation strategies:
- Approximation:
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- Nonlinearity - use tailored synthetic inputs:
  - E.g., choose values to make denominators $O(1)$
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1. Approximation:
   - Test the implementation not the math (i.e., duck)
   - 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

Consider the apparent contradiction:
TDD without “known” solutions

Consider the apparent contradiction:

- Complex algorithms yield few nontrivial analytic solutions.
- Implementations are not random keystrokes
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How can this be?

- Apparently analytic solutions are unnecessary!
- Algorithms are only sequences of steps
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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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TDD and irreducible complexity

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- Long answer: Well, they shouldn’t be ...
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  - Models couple many components/algorithms ⇒ exponential complexity
  - Tests are decoupled ⇒ linear complexity
TDD and emergent properties

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  2. Coupling/compositions have defects $\Rightarrow$ add tests
  3. System lacks sufficient accuracy $\Rightarrow$ increase accuracy
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  - Insufficient physical fidelity - science issue (testing is not magic)
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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
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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

Tom Clune
Thomas.L.Clune@nasa.gov
http://pfunit.sourceforge.net

Test-Driven Development: By Example - Kent Beck