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
Motivation 1: Fear/Stress

photomatt7.wordpress.com
Motivation 1: Fear/Stress
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Motivation 2: Productivity
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- New feature
- Refactor

Change
Verify
Motivation 2: Productivity

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- Compiles?
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Change - Verify

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- Really correct?
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Change

Verify

- Compiles?
- Executes?
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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

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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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  - No STDOUT; temp files deleted; ...
  - Order of tests has no consequence.
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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
    
    ```python
    call assertEqual(120, factorial(5))
    ```
  - Register test procedures with framework
  - Execute test procedures, and summarize success/failure

- Report: 1271 tests run 2 Failures
Testing Frameworks

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

- Tests written by separate team (black box testing)
- 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

Success? (Pass/Fail)

Focus on interface
Focus on algorithm

Refactor
Benefits of TDD

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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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- Presence of numerical error (roundoff or truncation)
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- 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 asymptotic form with unknown leading coefficient!
TDD techniques in presence of numerical error
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1. Approximation
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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
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- Nonlinearity - use tailored synthetic inputs:
  - E.g., choose values to make denominators $O(1)$
- 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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- Short answer: **No**
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
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  2. Coupling/compositions have defects ⇒ add tests
  3. System lacks sufficient accuracy ⇒ increase accuracy
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- Individual steps have defects ⇒ add unit tests
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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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- 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

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Test-Driven Development: By Example - Kent Beck