Test Driven Development of Scientific Models

SEA Conference - April 7-11, 2014
Boulder, CO

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

Outline

Motivation 1: Fear/Stress

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photomatt7.wordpress.com

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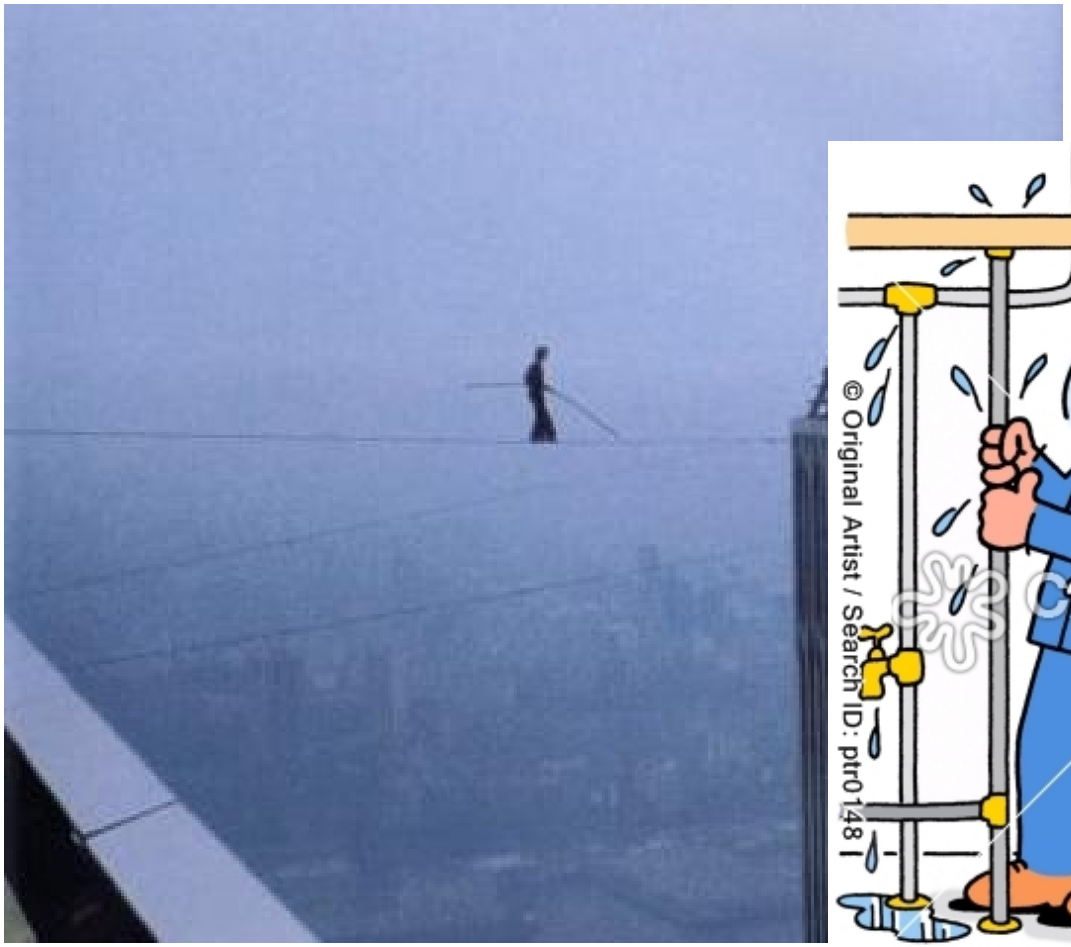

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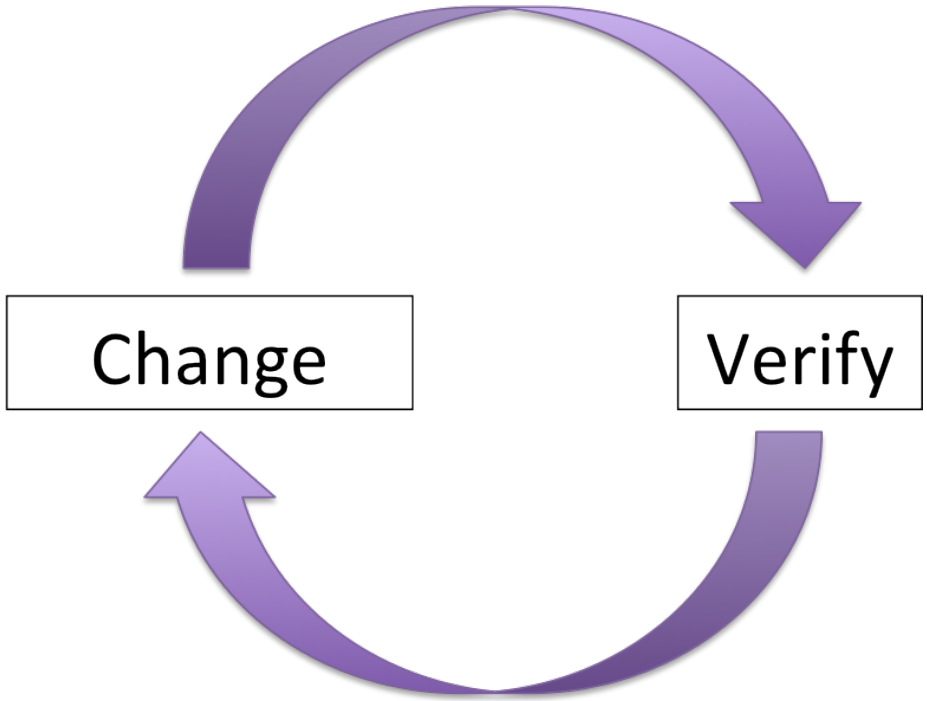
Motivation 1: Fear/Stress

Calvin & Hobbes - Bill Waterson

Motivation 2: Productivity



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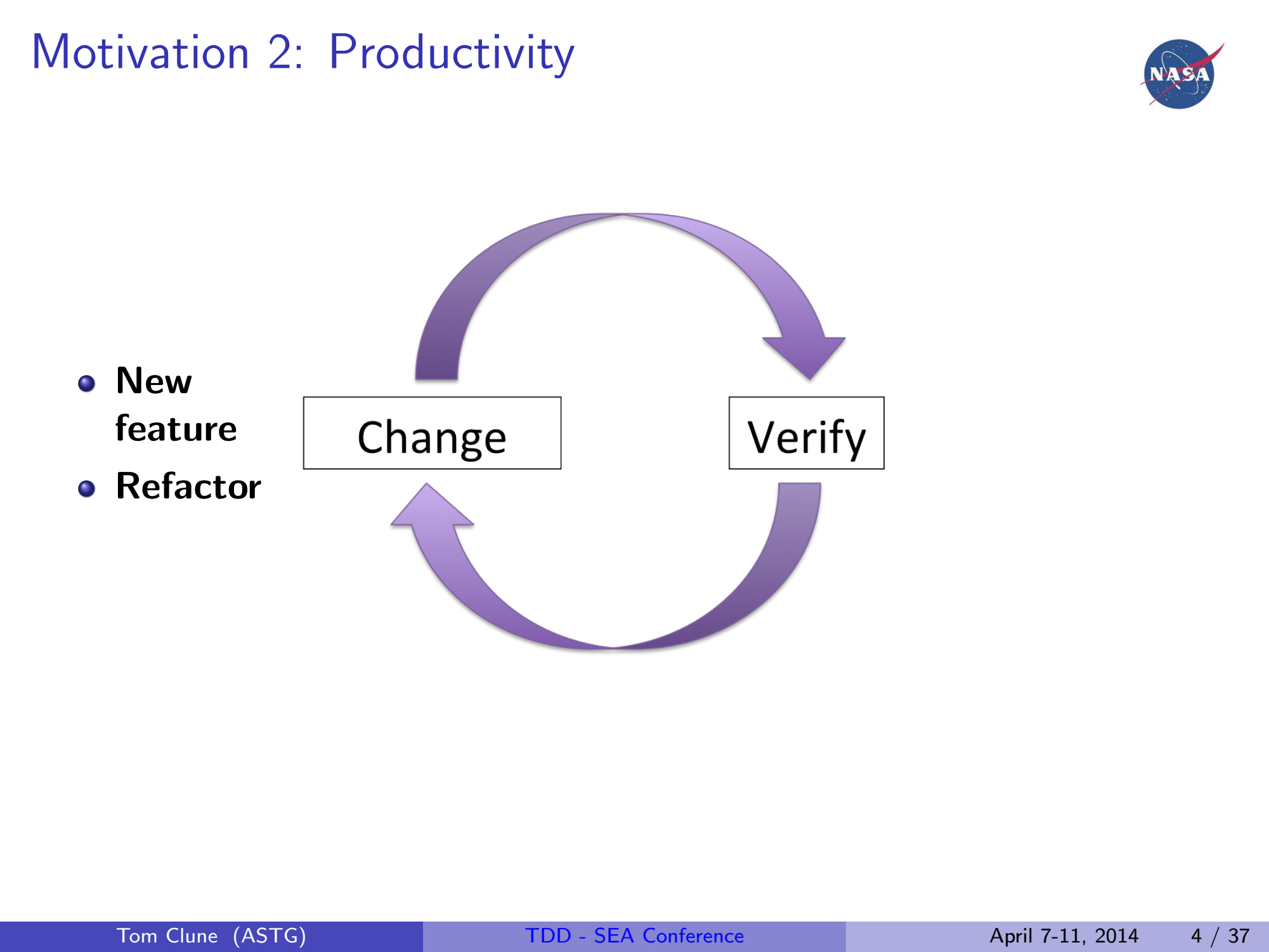

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- **Refactor**

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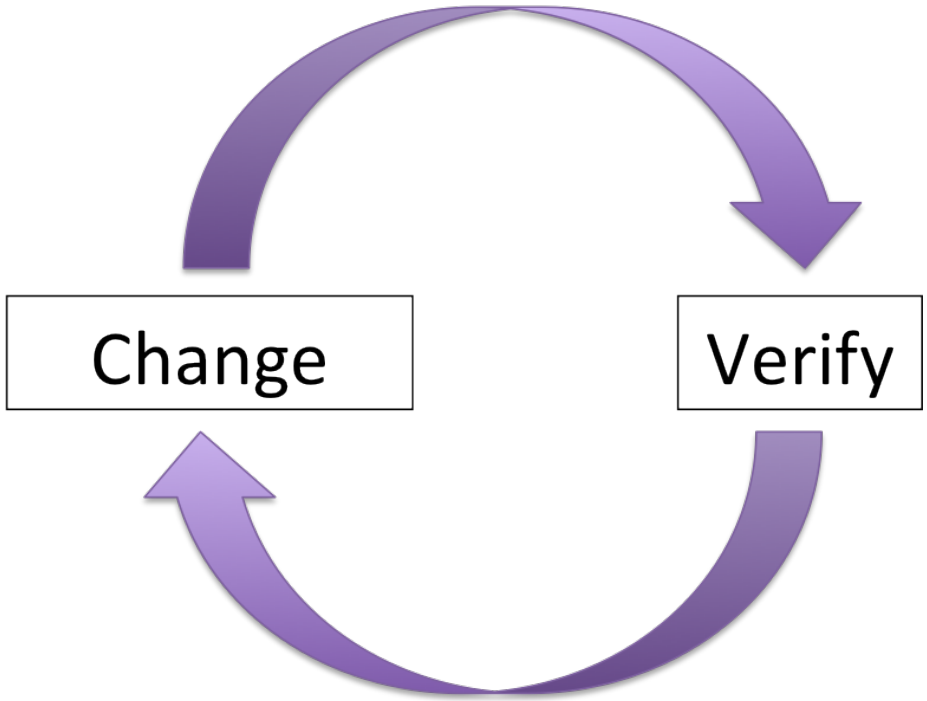

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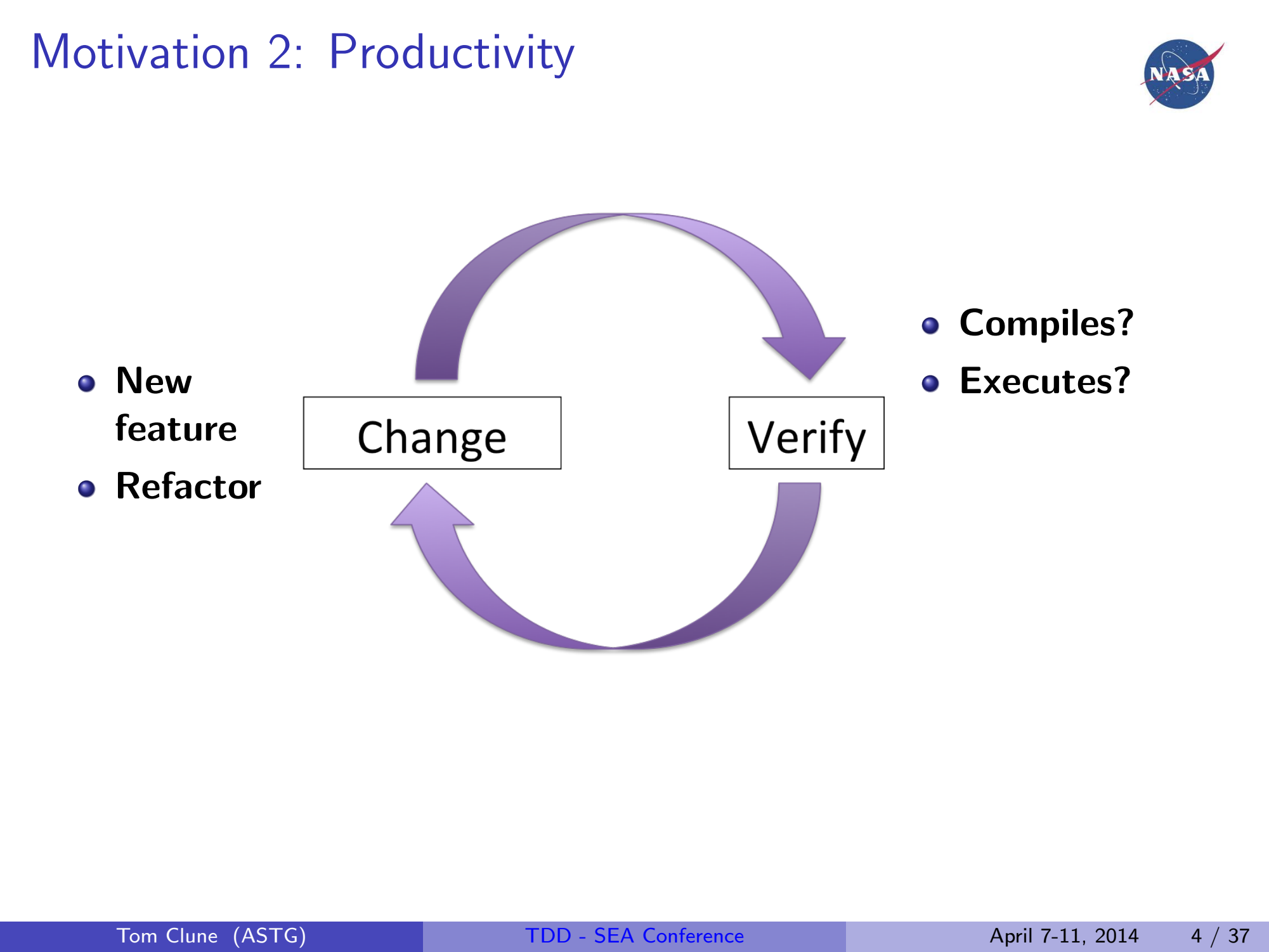

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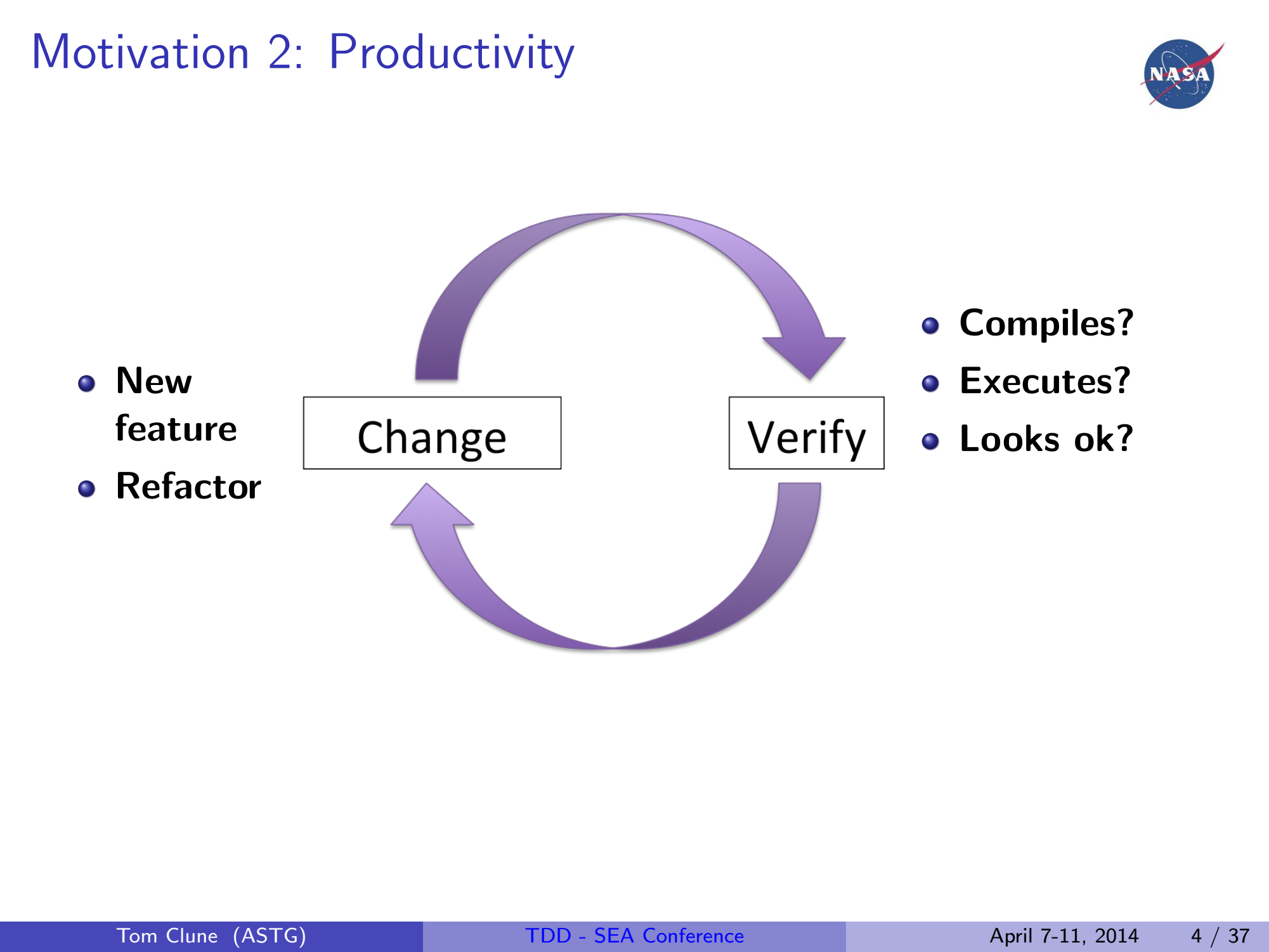

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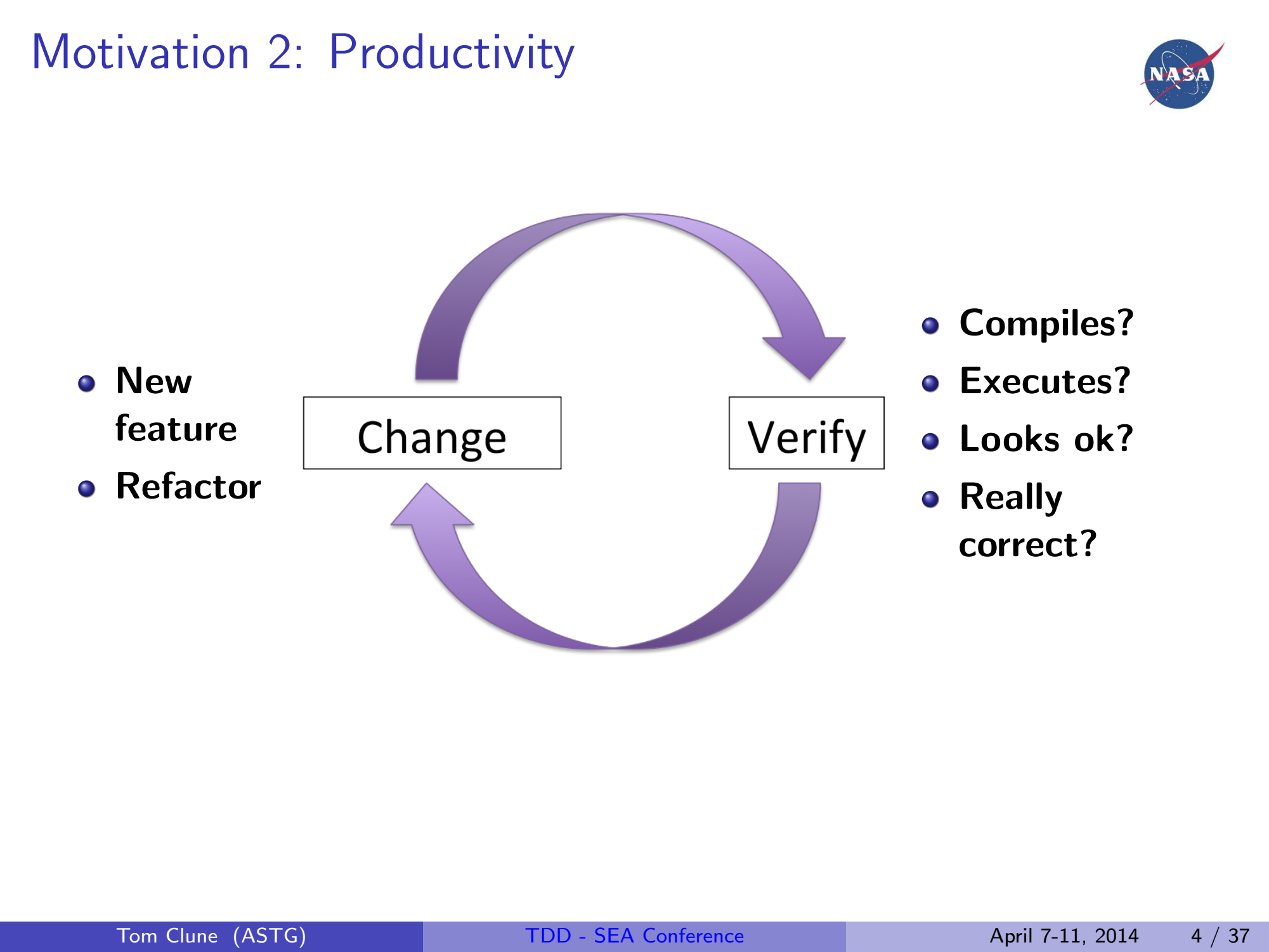

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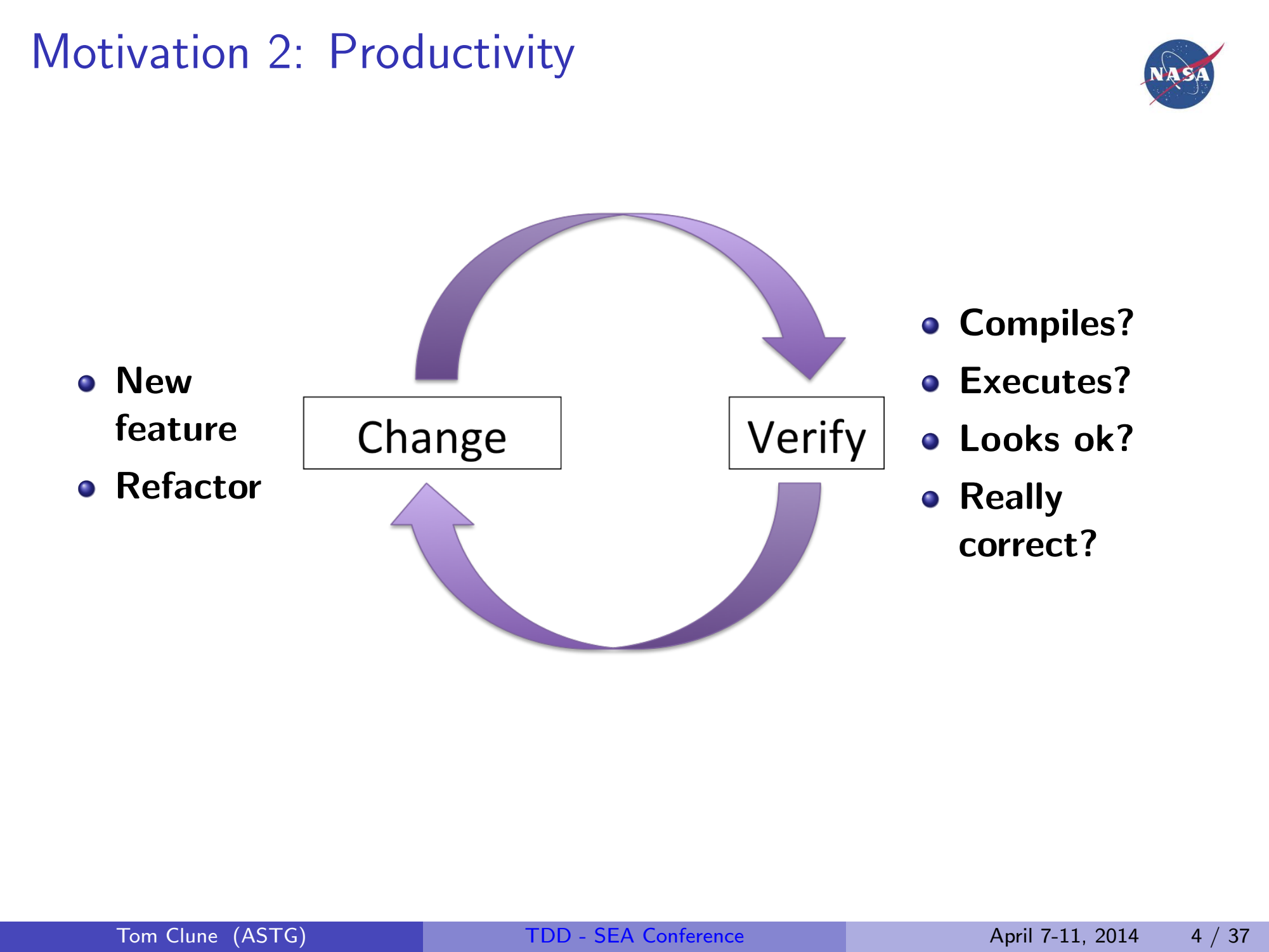

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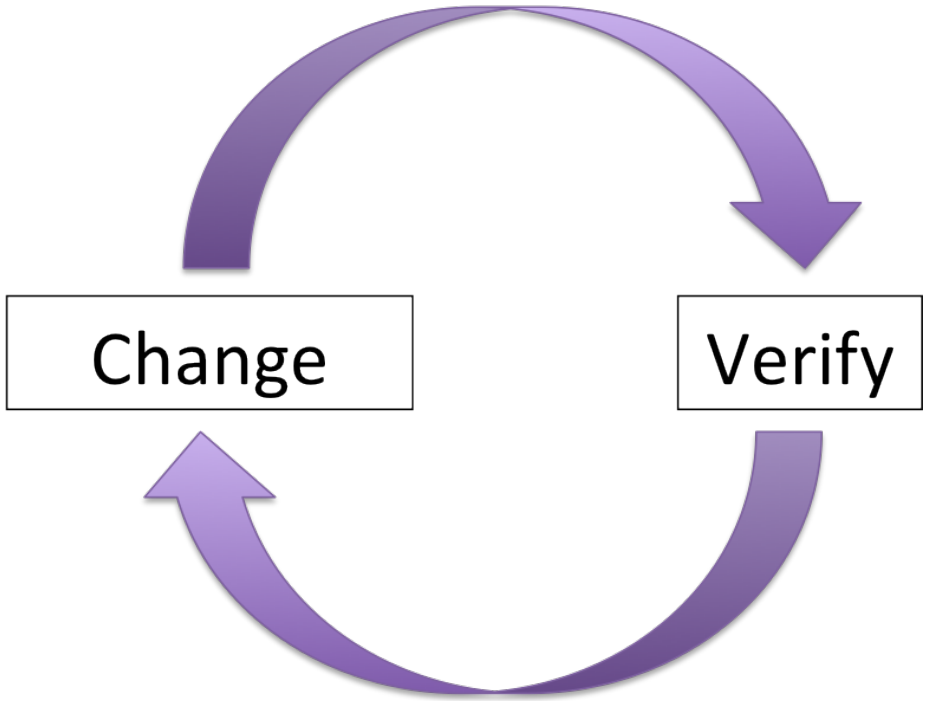

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What is the latency of verification for large scientific models?

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!

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  - ★ Those which change results below detection threshold

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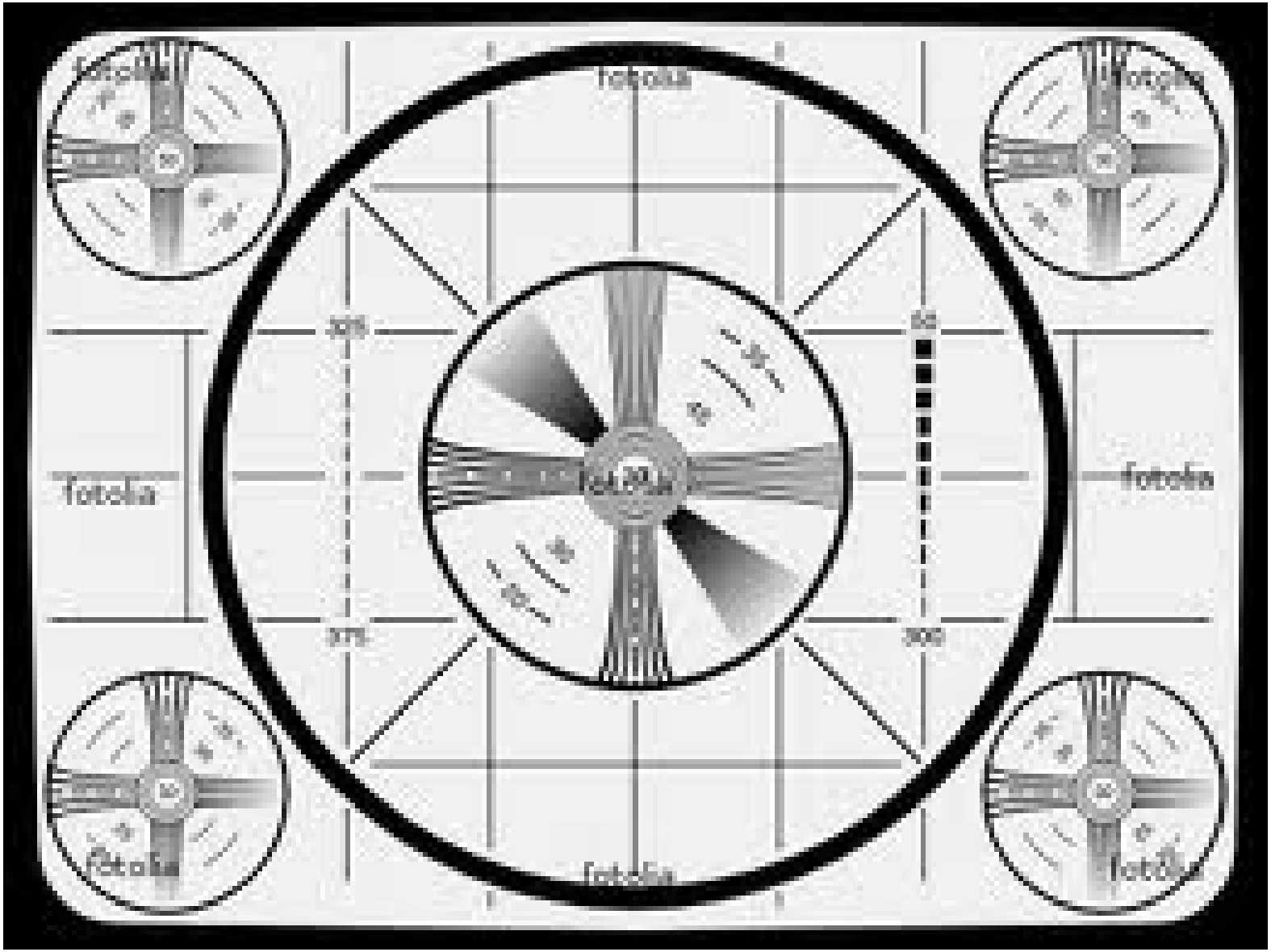
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- **Inexpensive compared to application (ideally)**

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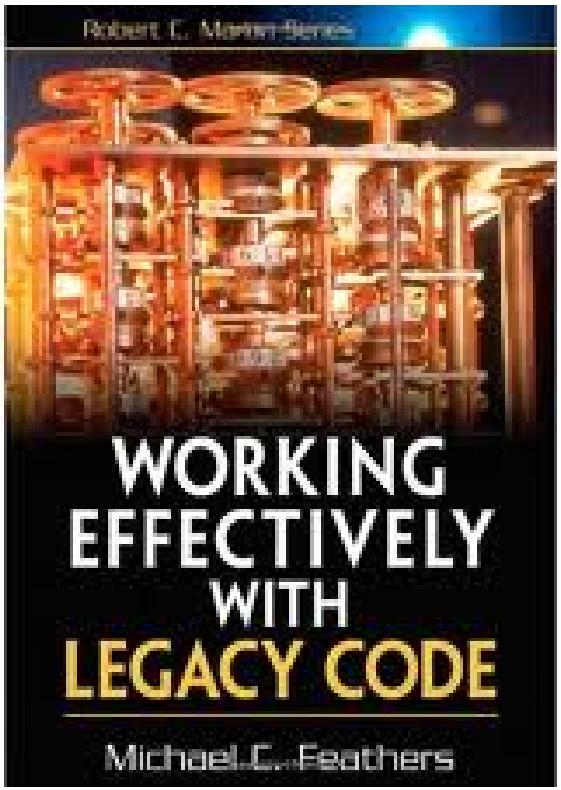

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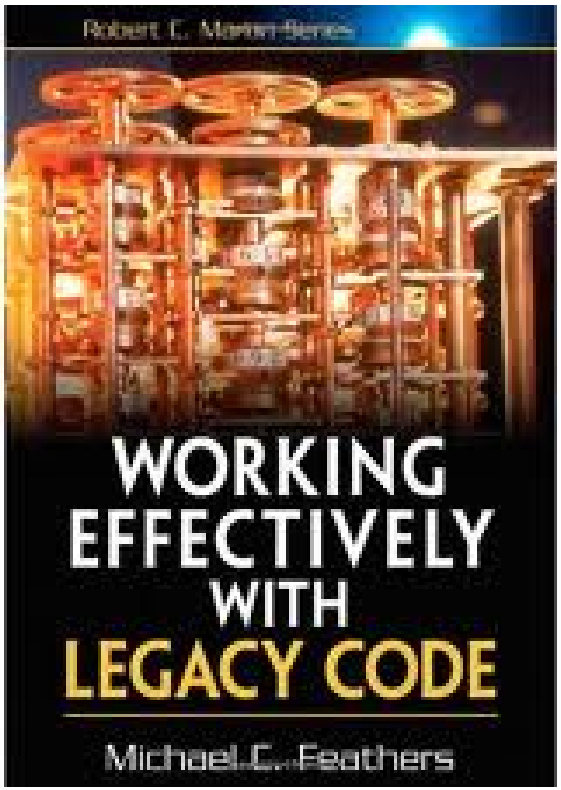

"Fear is the path to the dark side. Fear leads to anger. Anger leads to hate. Hate leads to suffering." - Yoda

starwars.wikia.com

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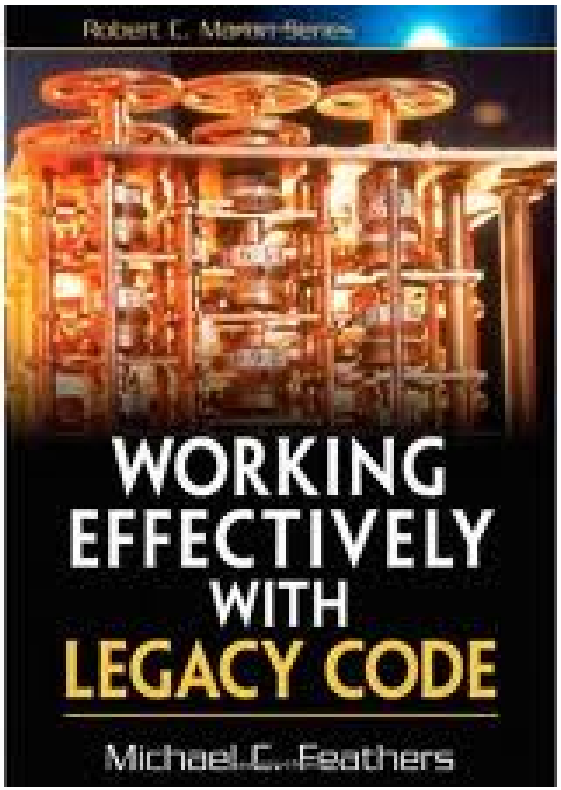

- Lack of tests leads to fear of introducing subtle bugs and/or changing things inadvertently.
- Also is a barrier to involving pure software engineers in the development of our models.

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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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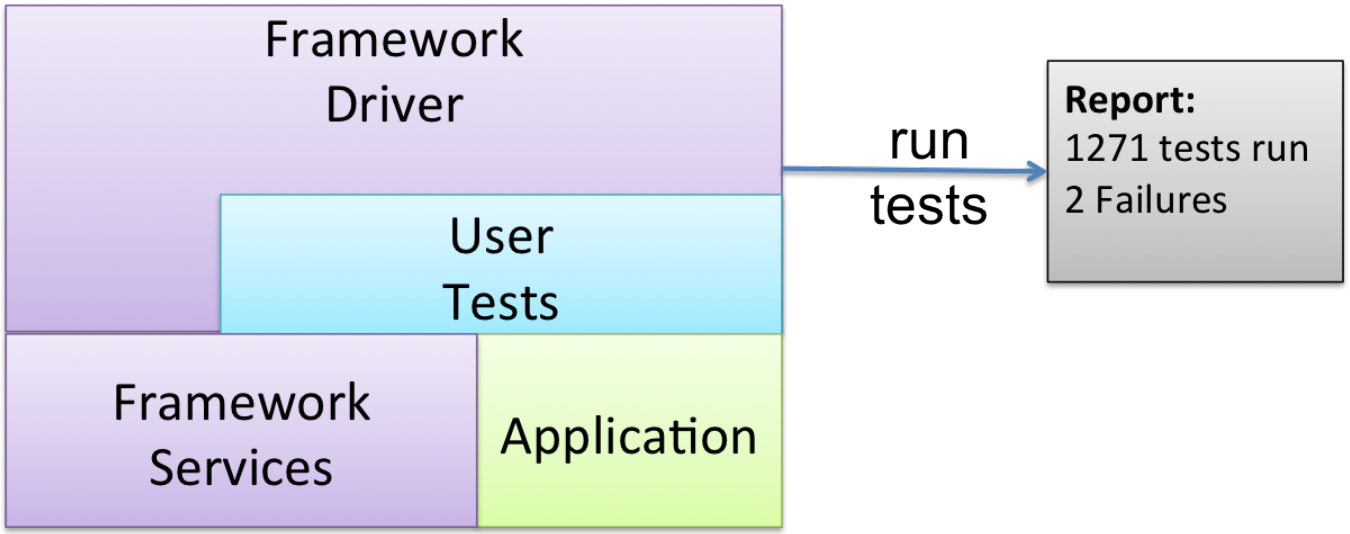
Testing Frameworks



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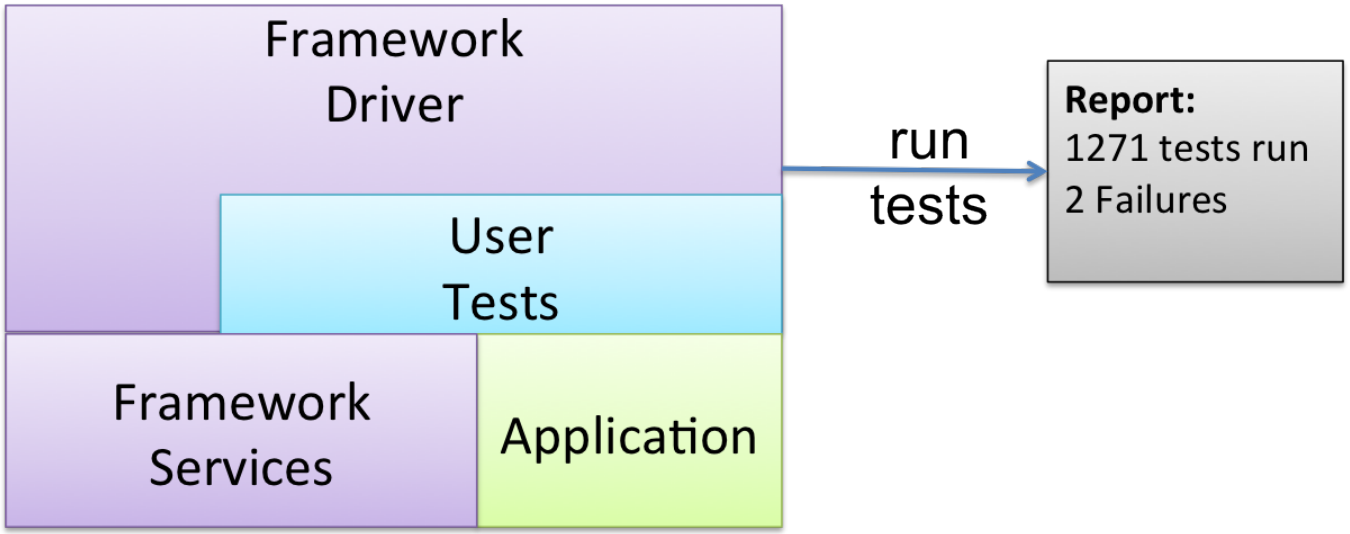

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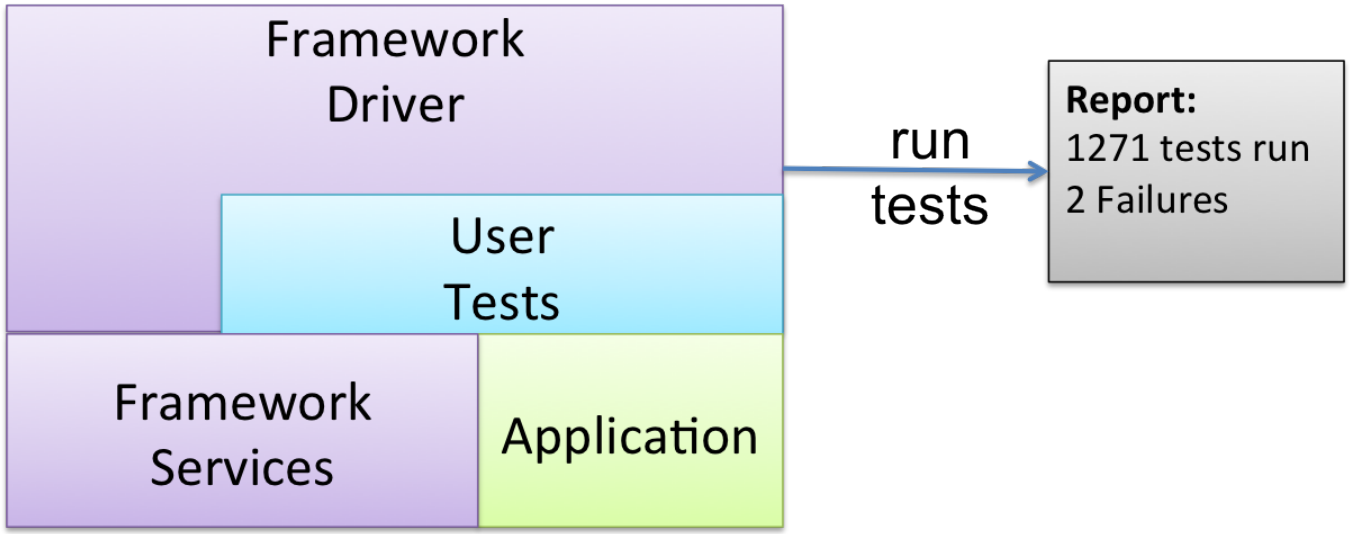

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  - Register test procedures with framework
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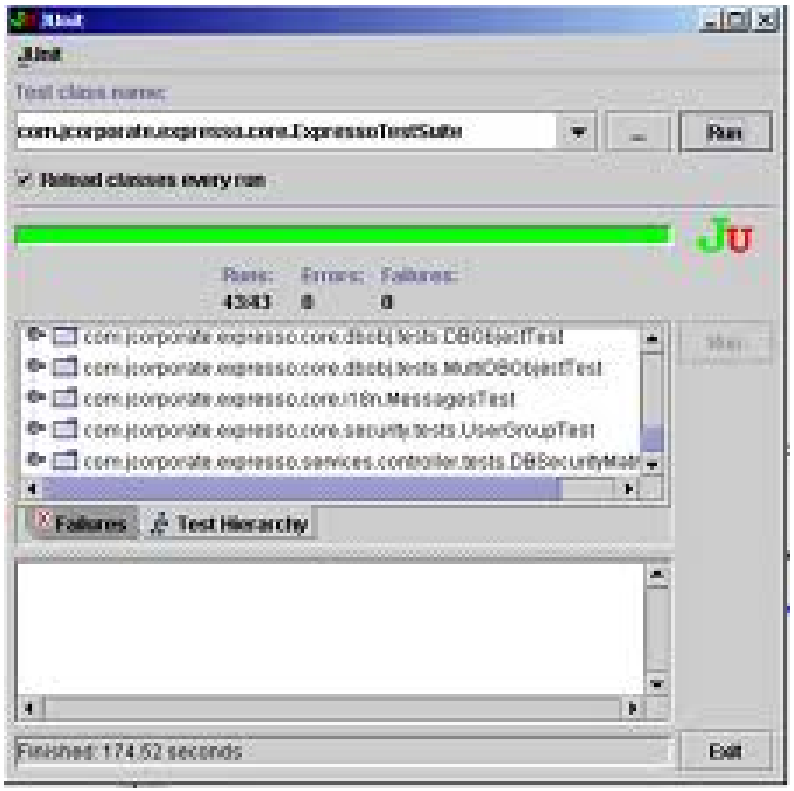
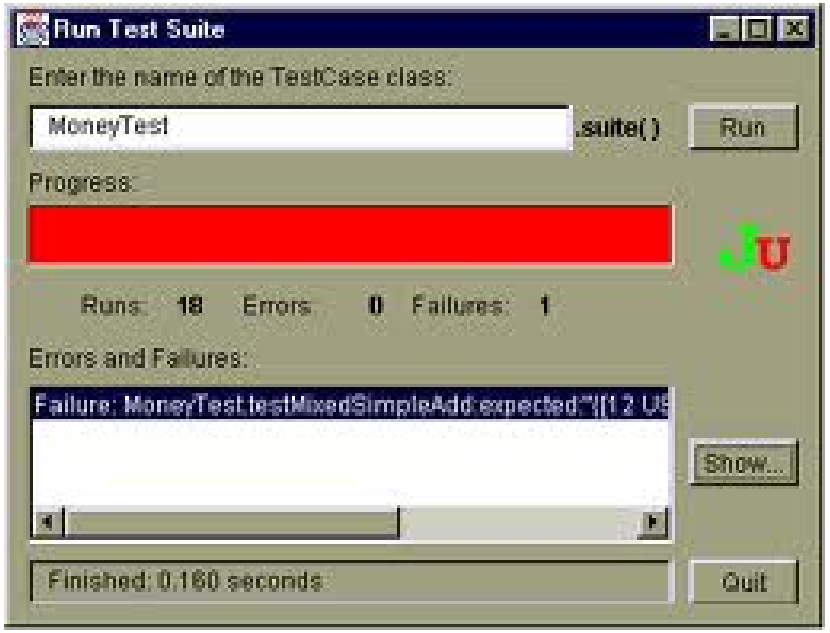
- Generally specific/customized to programming language (xUnit)
  - Java (JUnit)
  - Python (pyUnit)
  - C++ (cxxUnit, cppUnit)
  - Fortran (FRUIT, FUNIT, **pFUnit**)

Frameworks and IDE's

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





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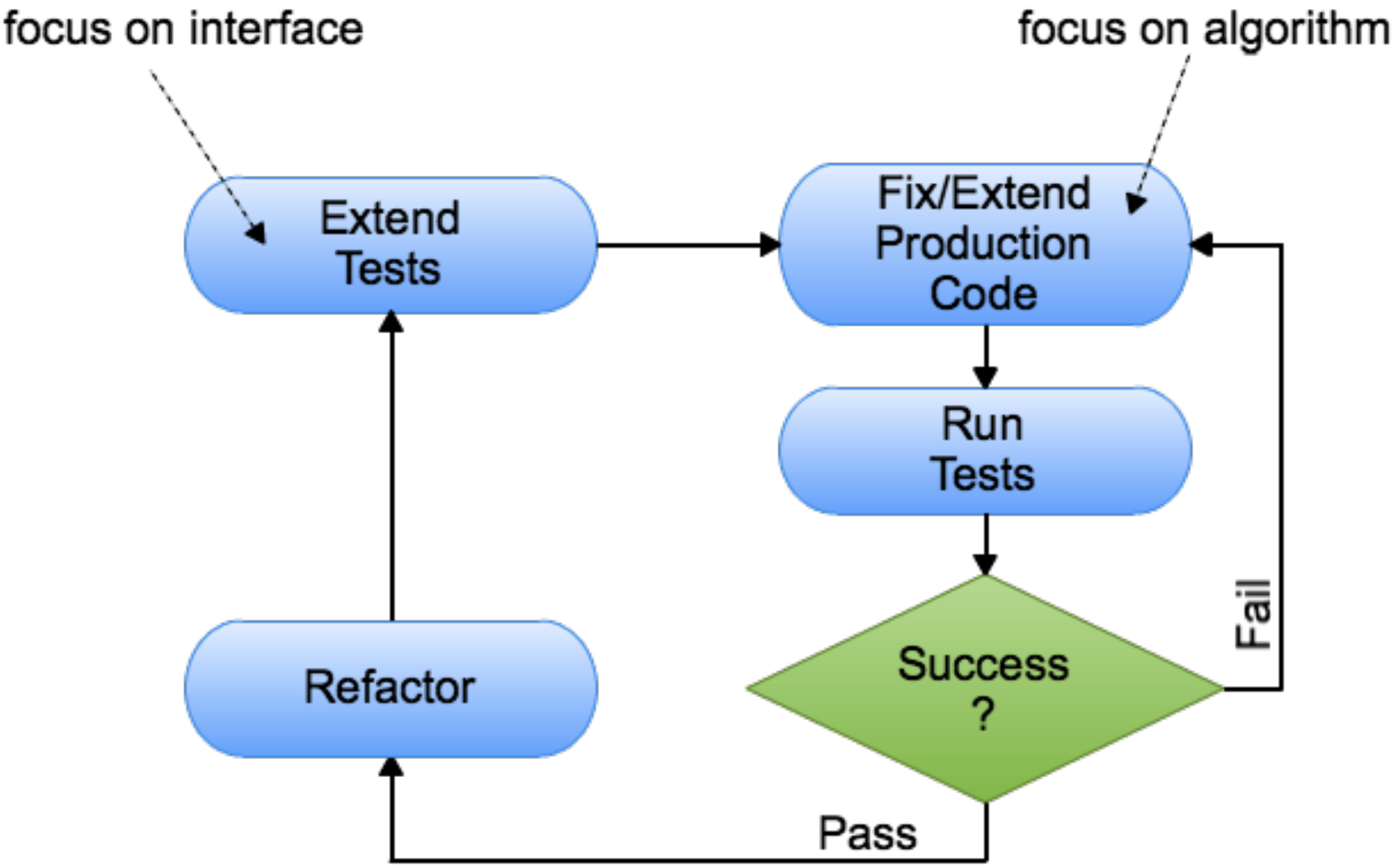
New paradigm - Test-driven development (TDD)

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

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2. Nonlinearity - use tailored synthetic inputs:
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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

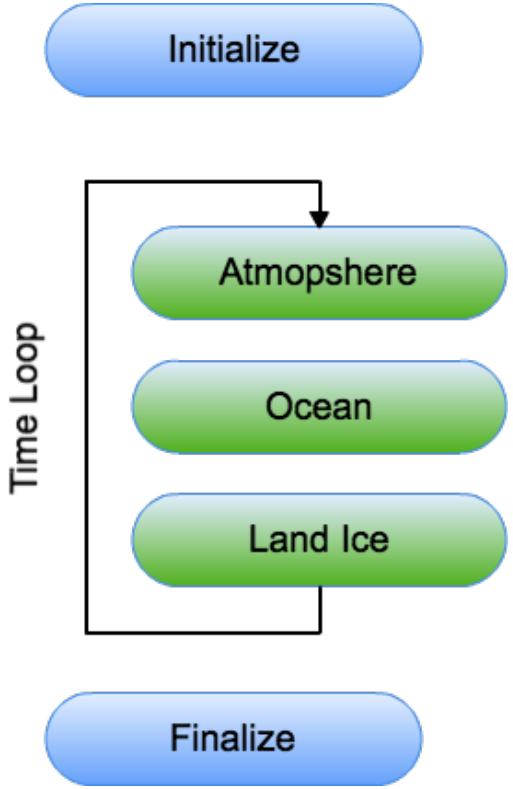
Consider the main loop of a climate model:

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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- Tailor synthetic inputs to yield "obvious" results for each step
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But still use high level analytic solutions as tests when available!

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  - Models *couple* many components/algorithms $\Rightarrow$ exponential complexity
  - Tests are *decoupled* $\Rightarrow$ linear complexity

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- 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

Acknowledgements

This work has been supported by

- NASA's High End Computing (HEC) program and
- NASA's Modeling, Analysis, and Prediction (MAP) Program.

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