Test Driven Development of Scientific Models

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Earth Science Division
NASA Goddard Space Flight Center

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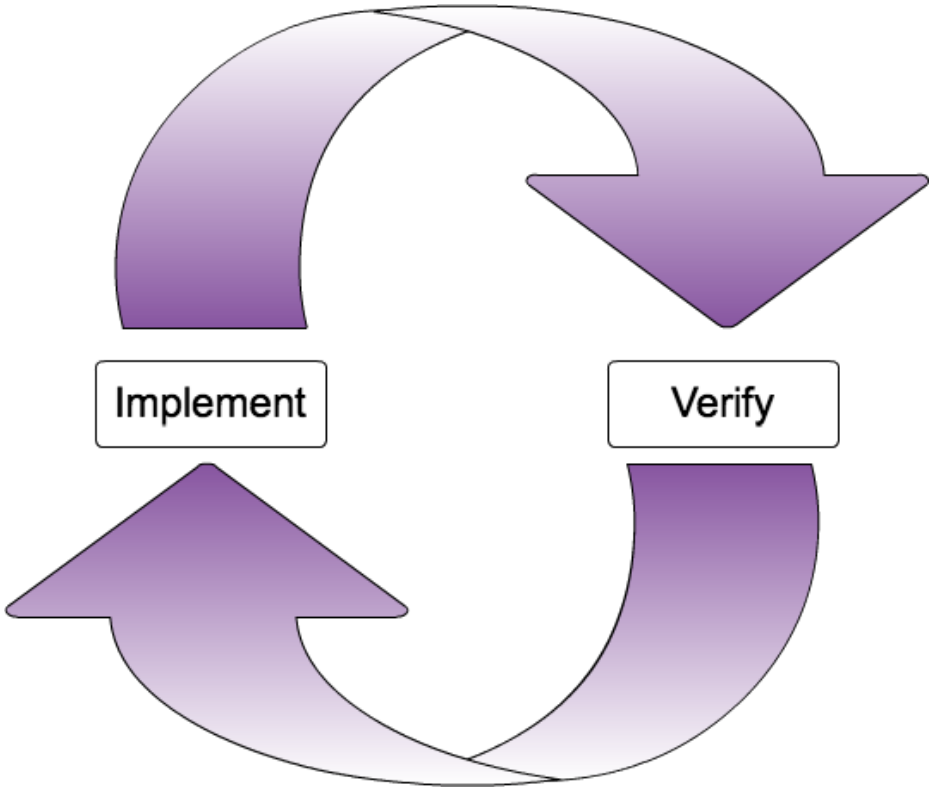
Outline

The development cycle and productivity



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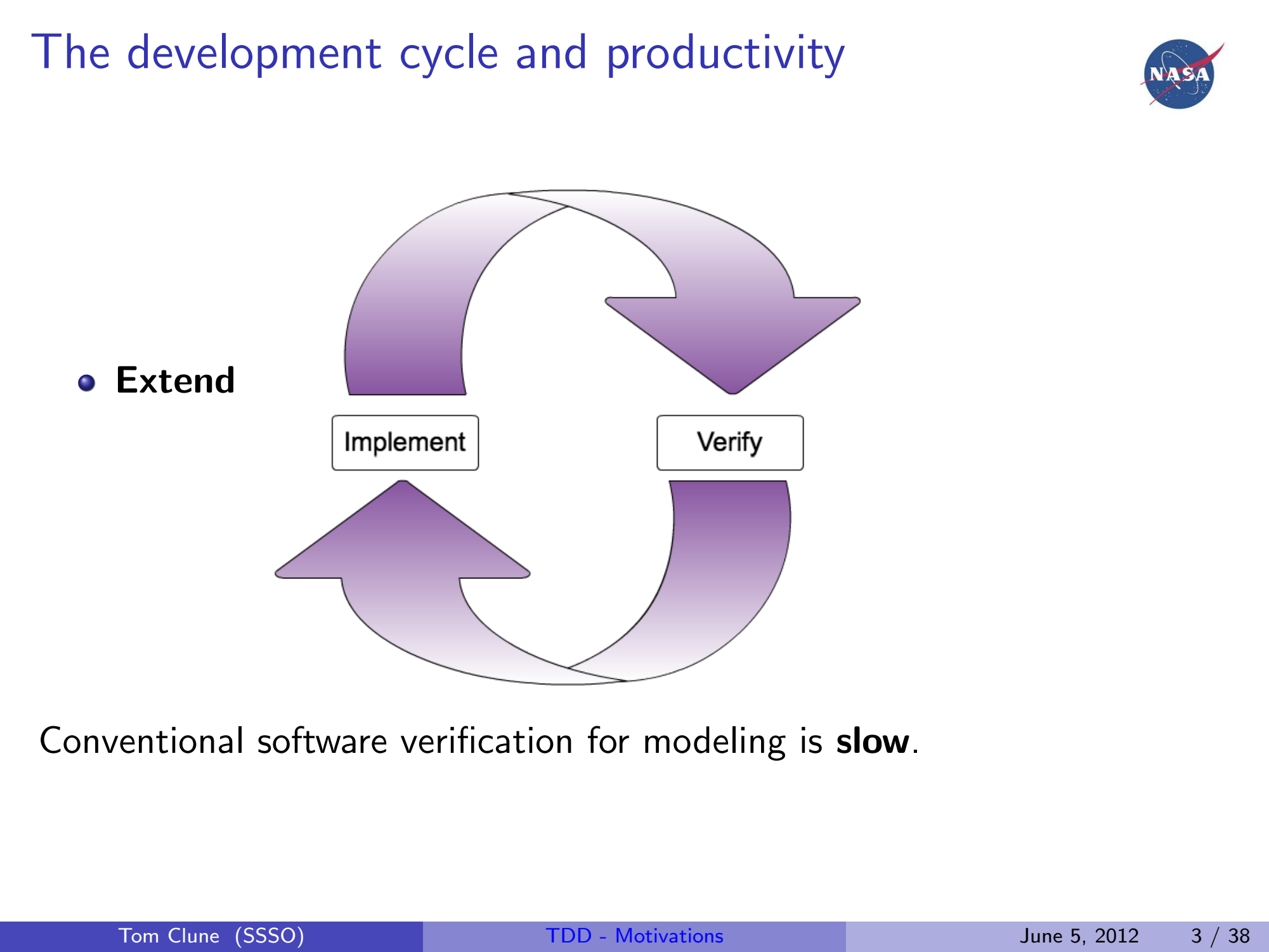

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Conventional software verification for modeling is **slow**.

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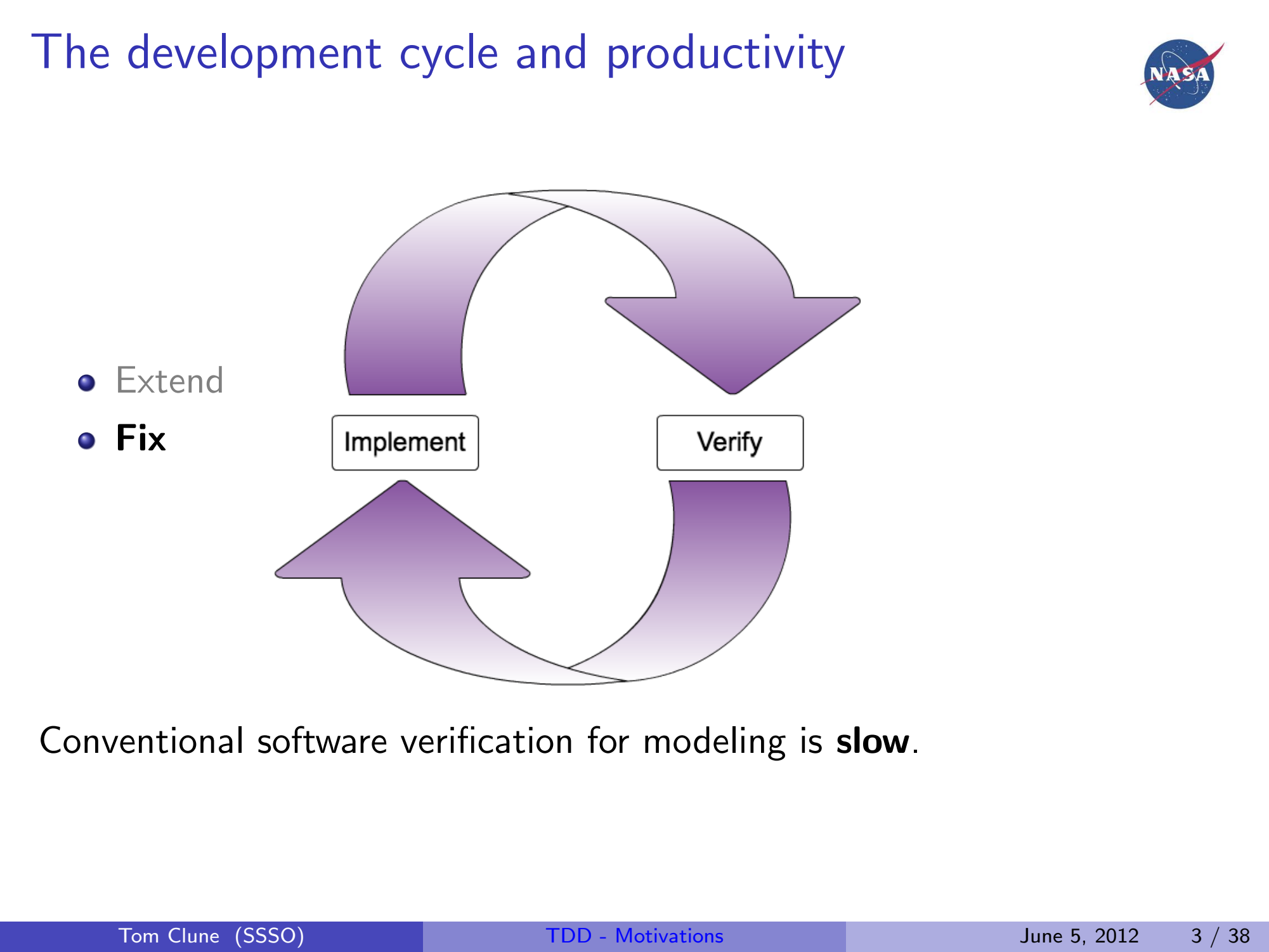

- Extend
- **Fix**

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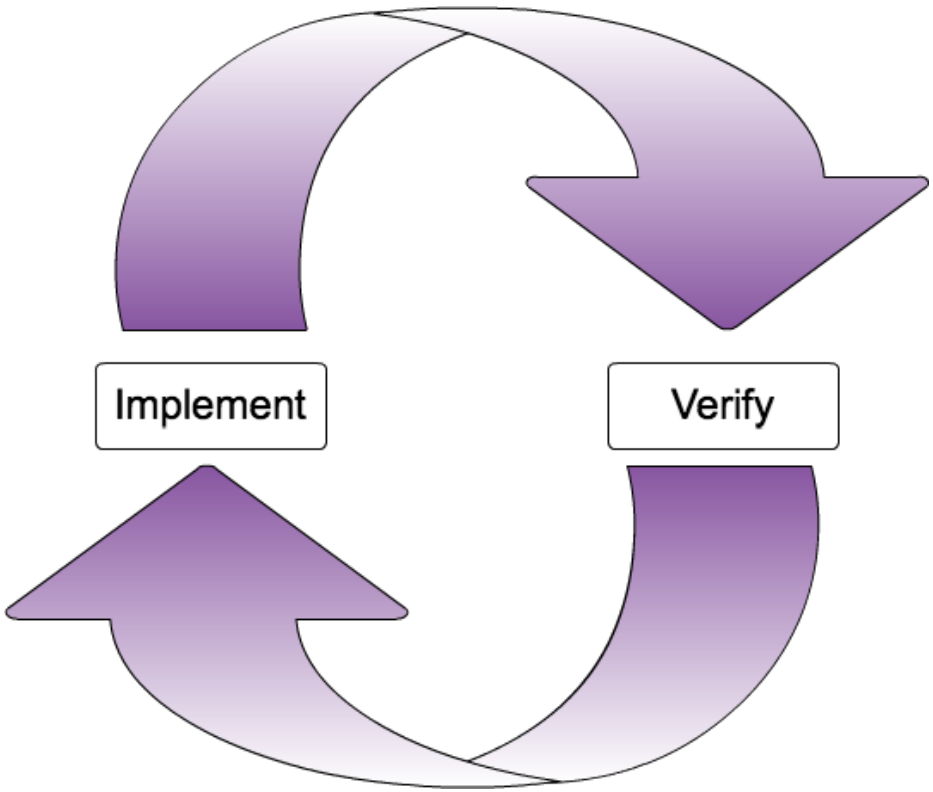
The development cycle and productivity

- Extend
- Fix
- **Port**



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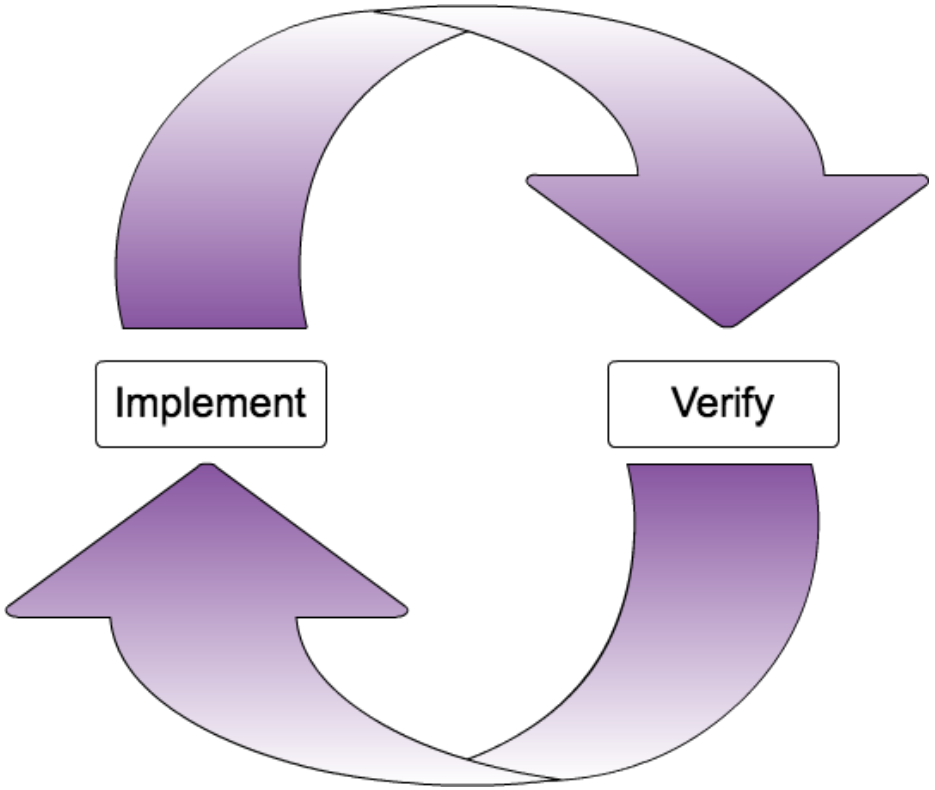

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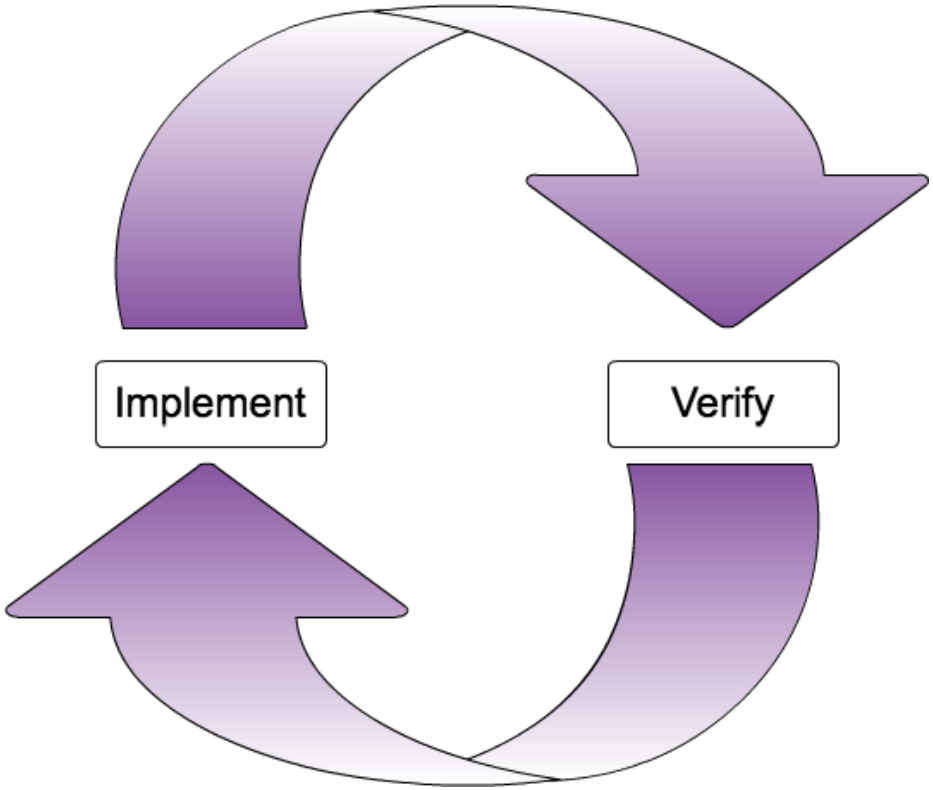

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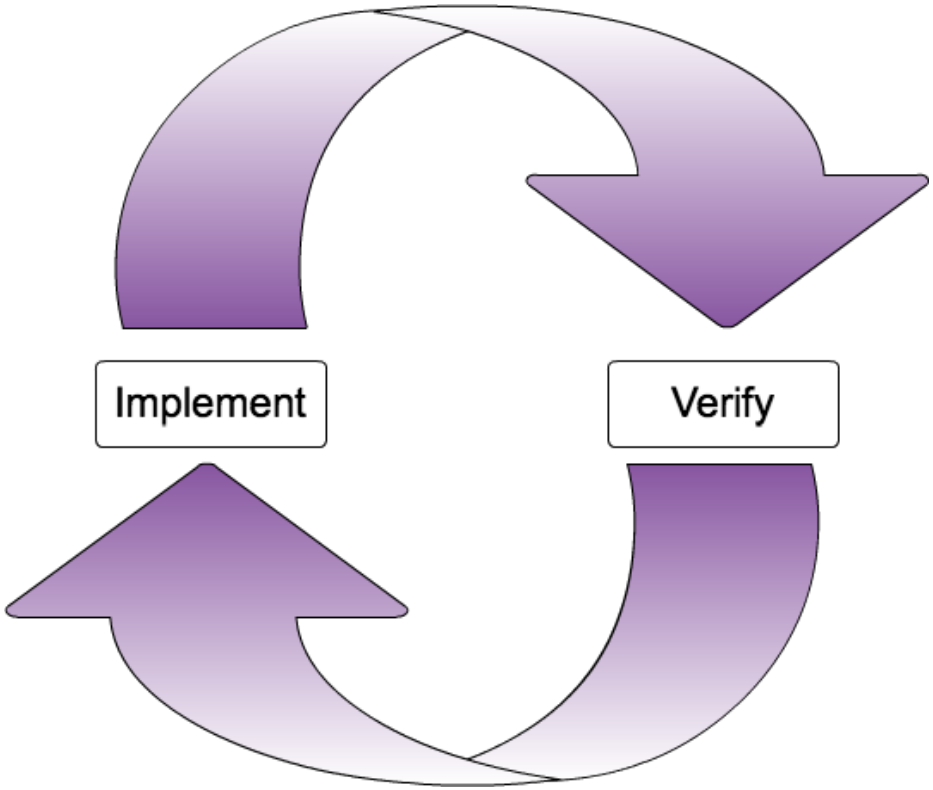

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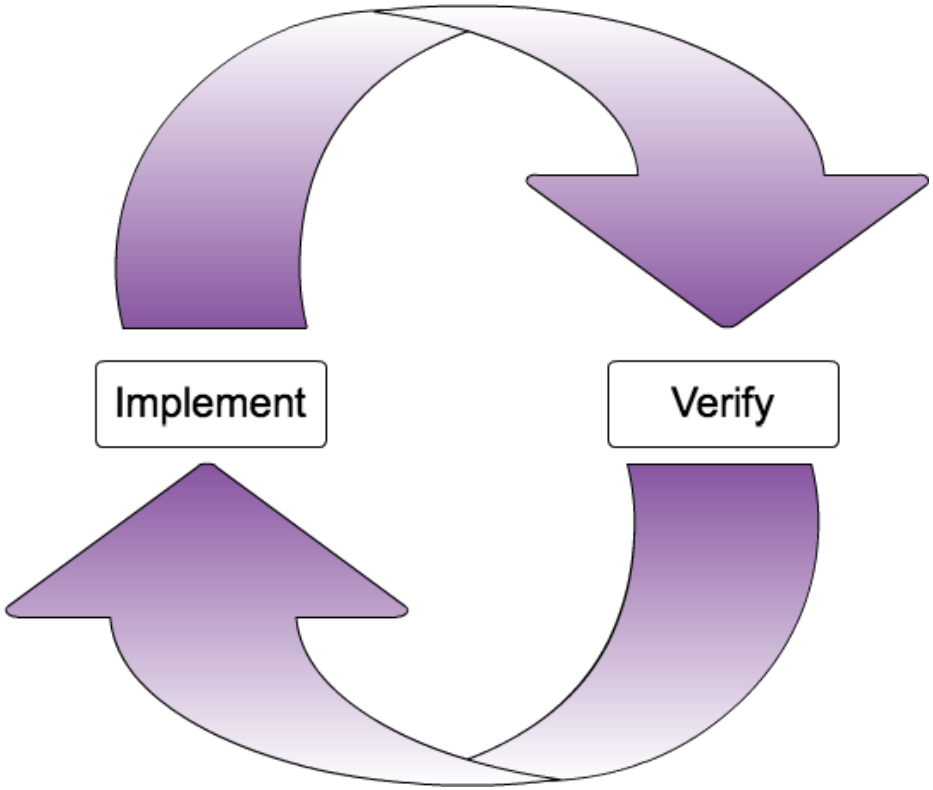

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- **Correct?**

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Some observations

- Risk grows with magnitude of implementation step
- Magnitude of implementation step grows with cost of verification/validation

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Conclusion:
Optimize productivity by reducing cost of verification!

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  - ★ Those which change results below detection threshold

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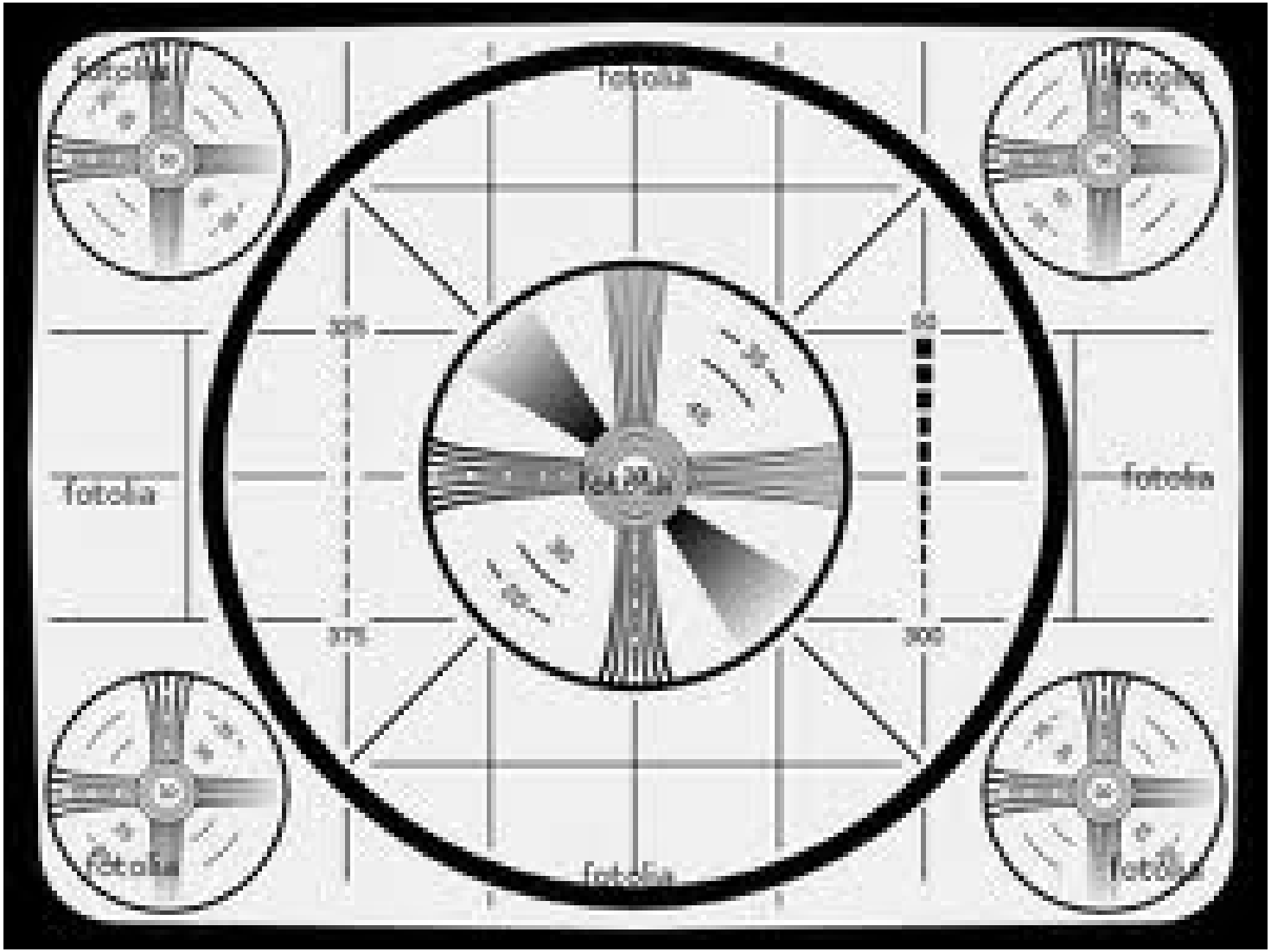
Testing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Test Harness - work in safety

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- Improves developer confidence
- **Decreases risk from change**

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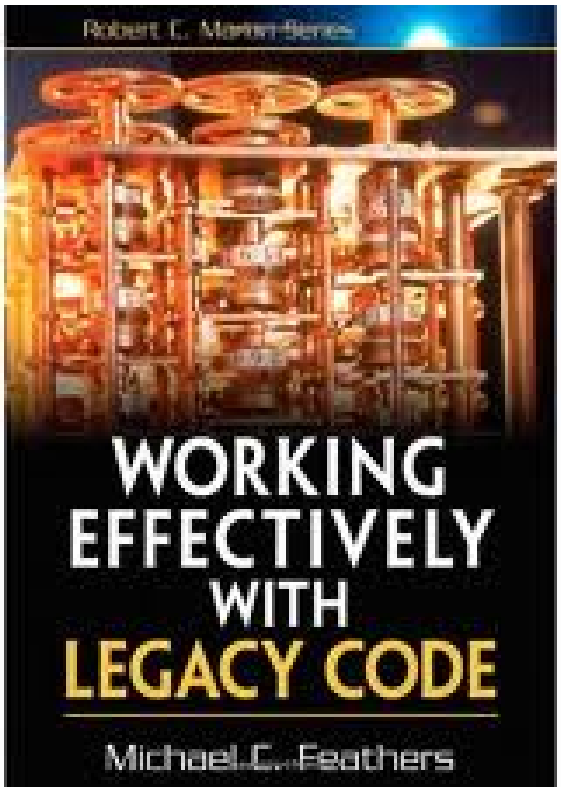
Working Effectively with Legacy Code



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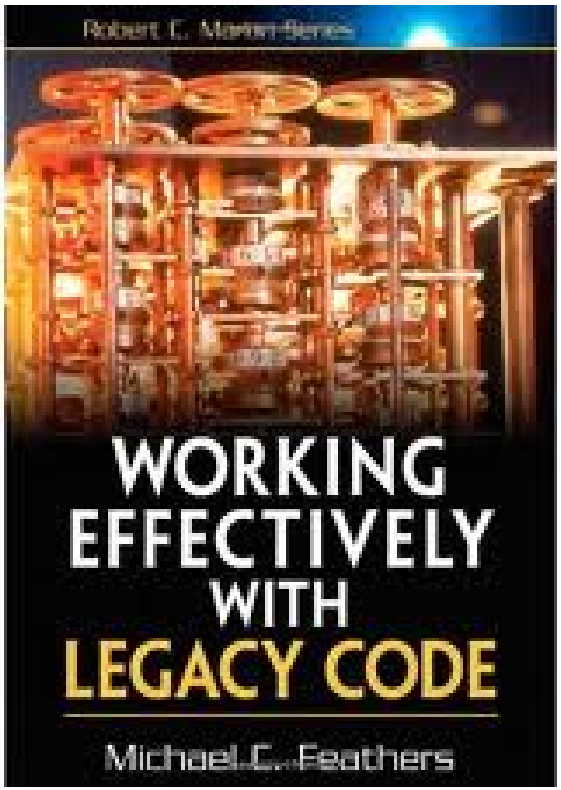

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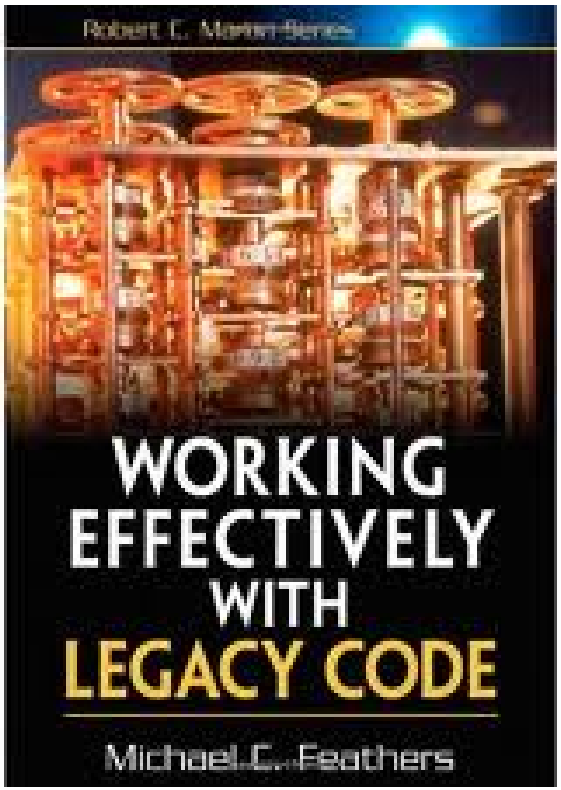

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This is also a barrier to involving pure software engineers in the development of our models.

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

Just what is a test anyway?

Tests can exist in many forms

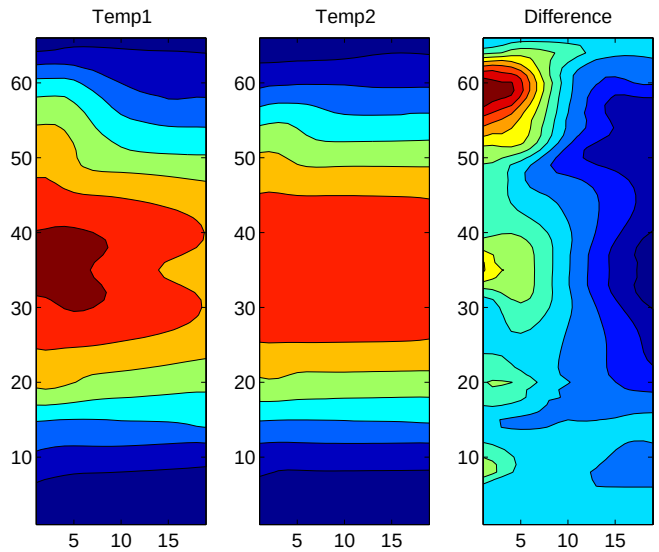
- Conditional termination:

```
IF (PA(I,J)+PTOP.GT.1200.) &
    call stop_model('ADVECM: Pressure diagnostic error',11)
```

- Diagnostic print statement

```
print*, 'loss of mass = ', deltaMass
```

- Visualization of output



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Design experiment	$\longrightarrow$	Write a test
Run experiment	$\longrightarrow$	Run tests
Refine hypothesis	$\longrightarrow$	Refine implementation

http://agile2003.agilealliance.org/files/P6Paper.pdf

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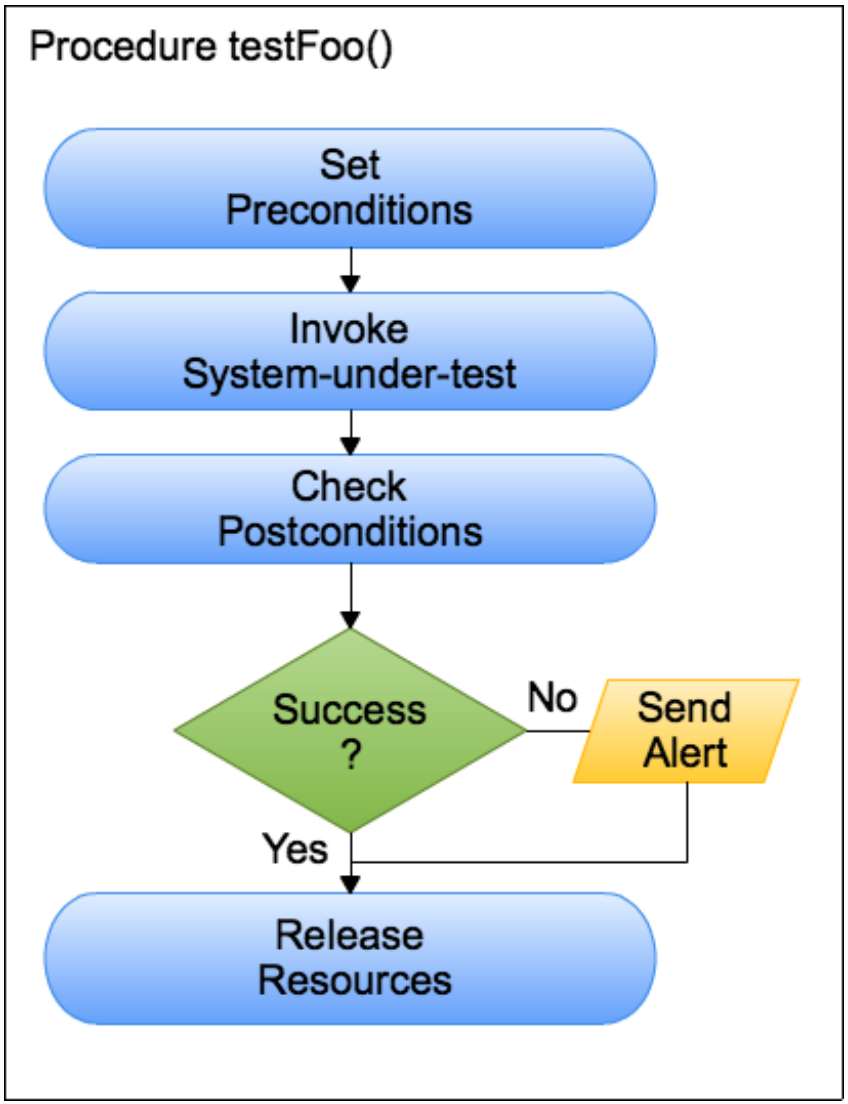

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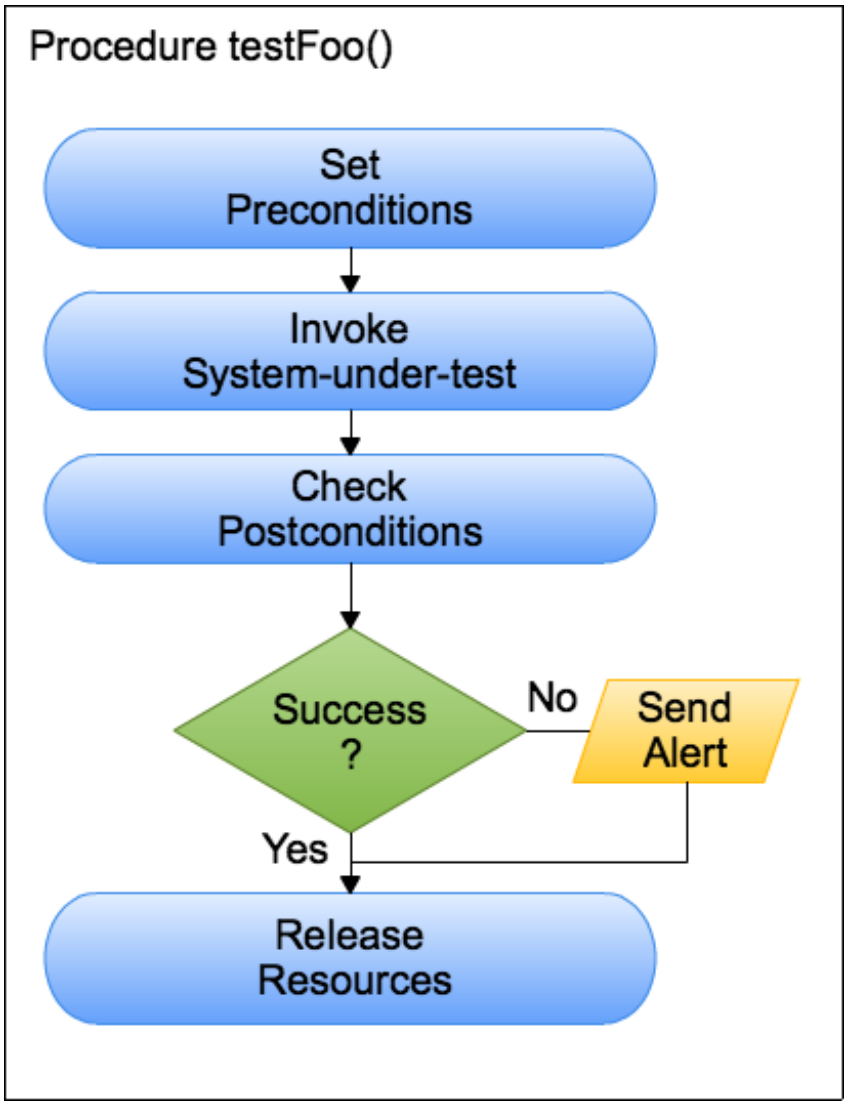

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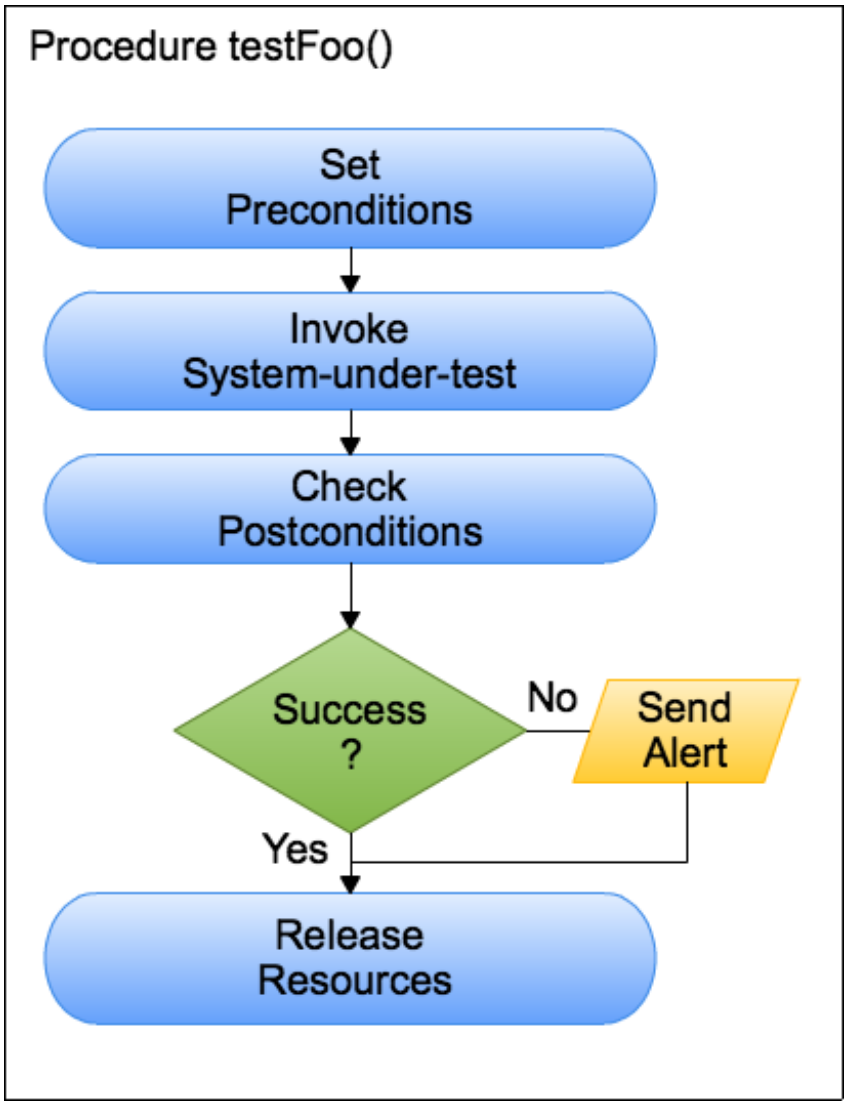

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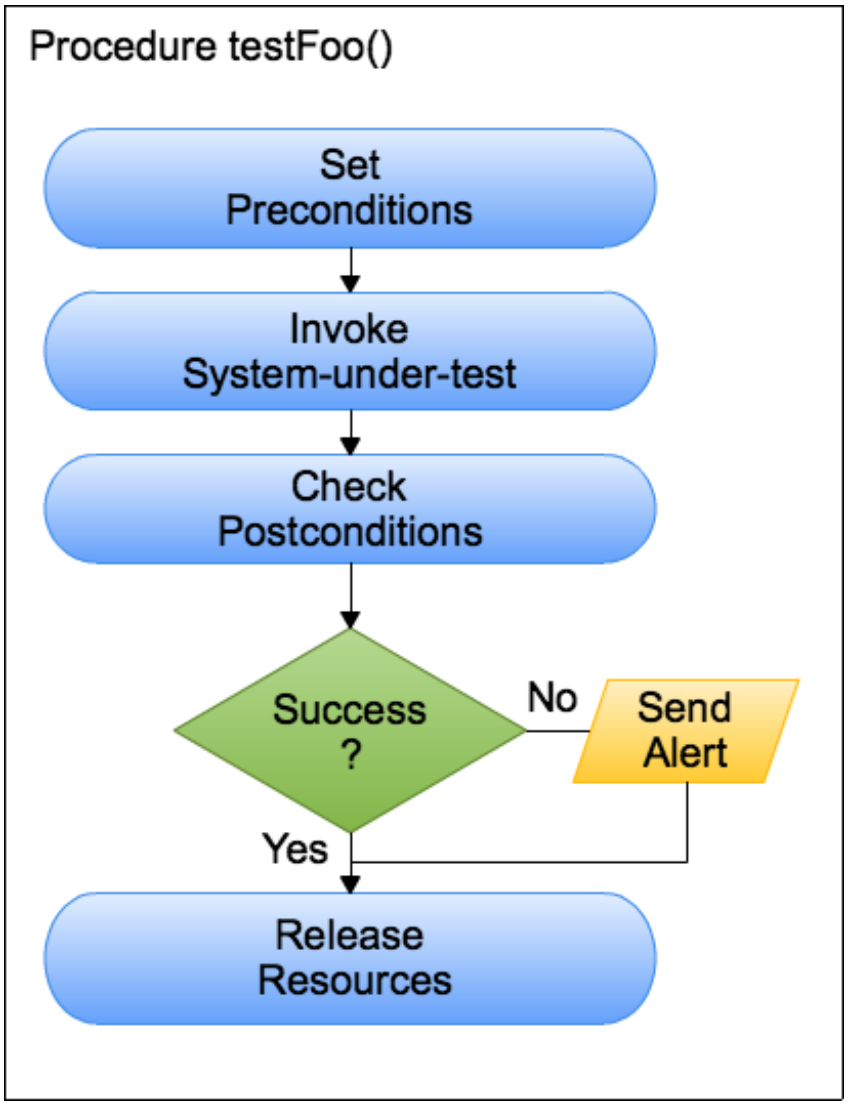

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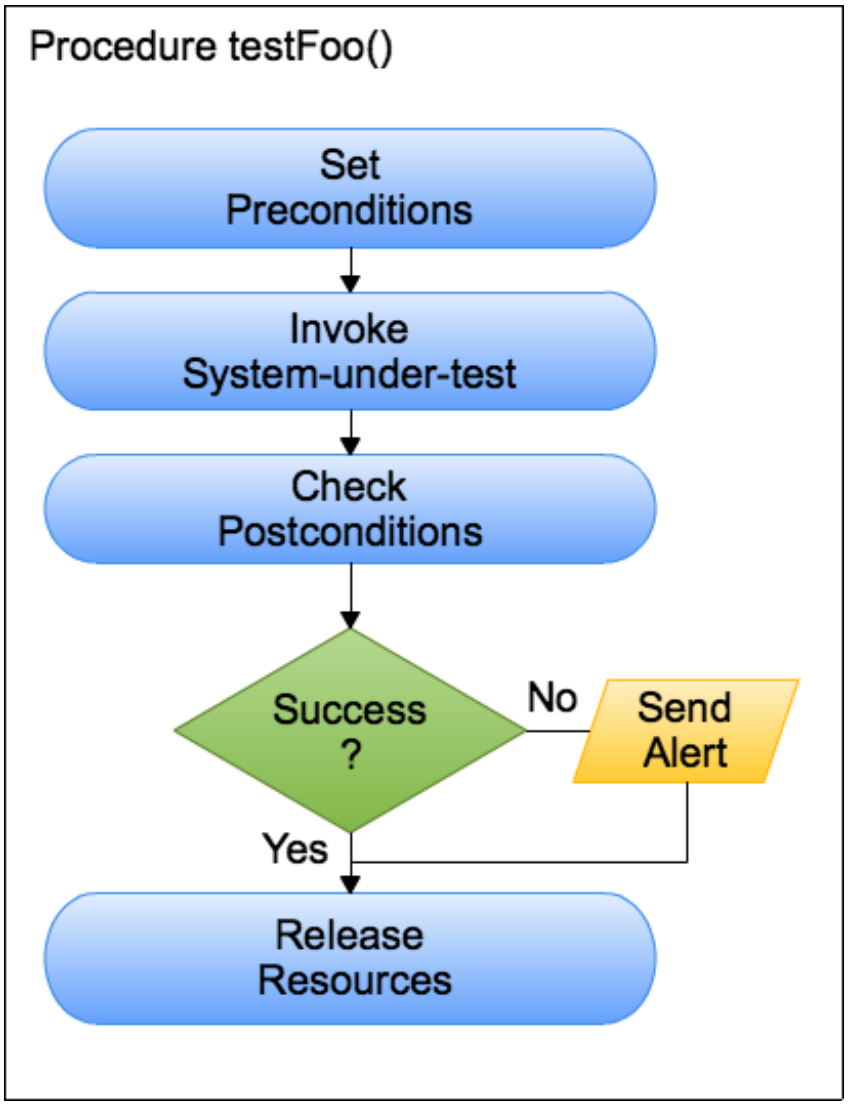

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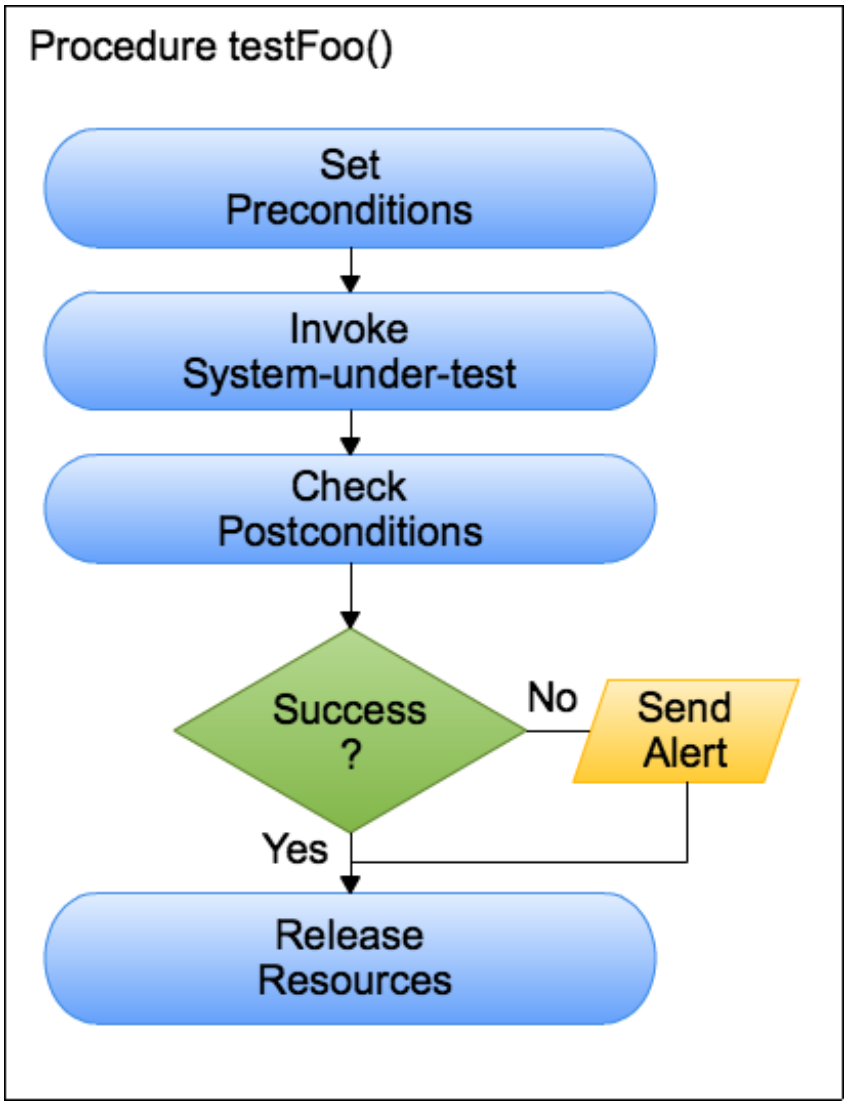

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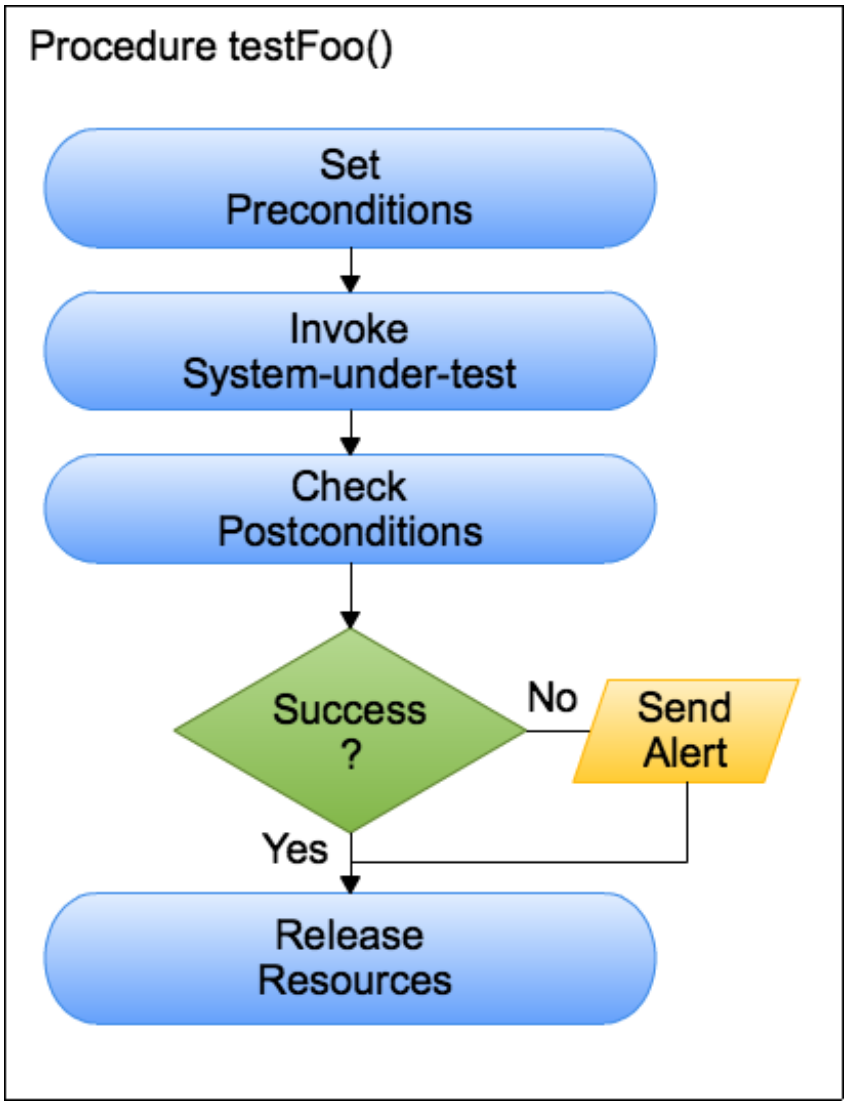

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Outline

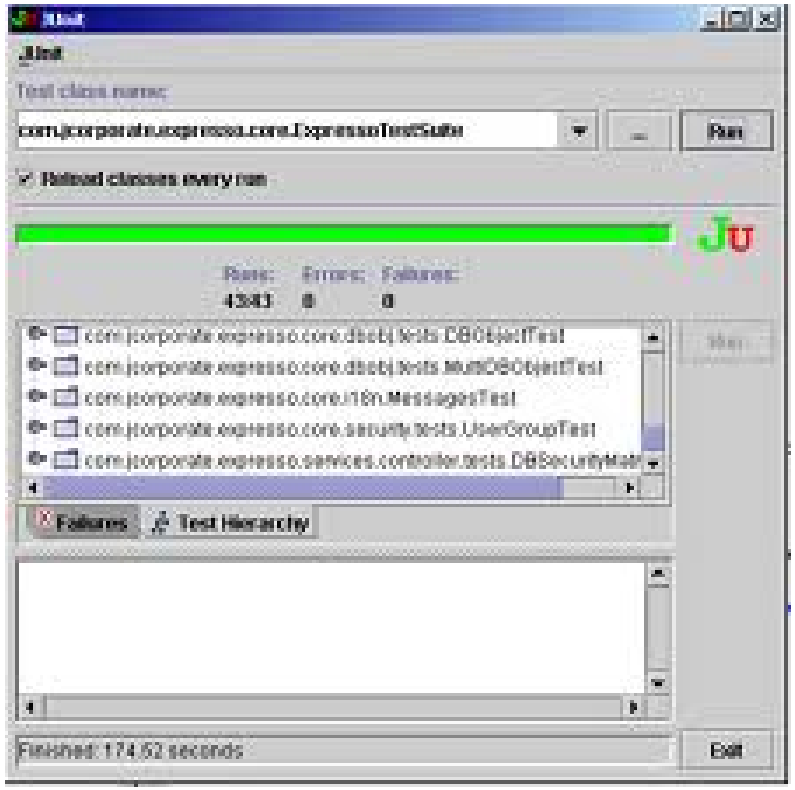
Testing Frameworks

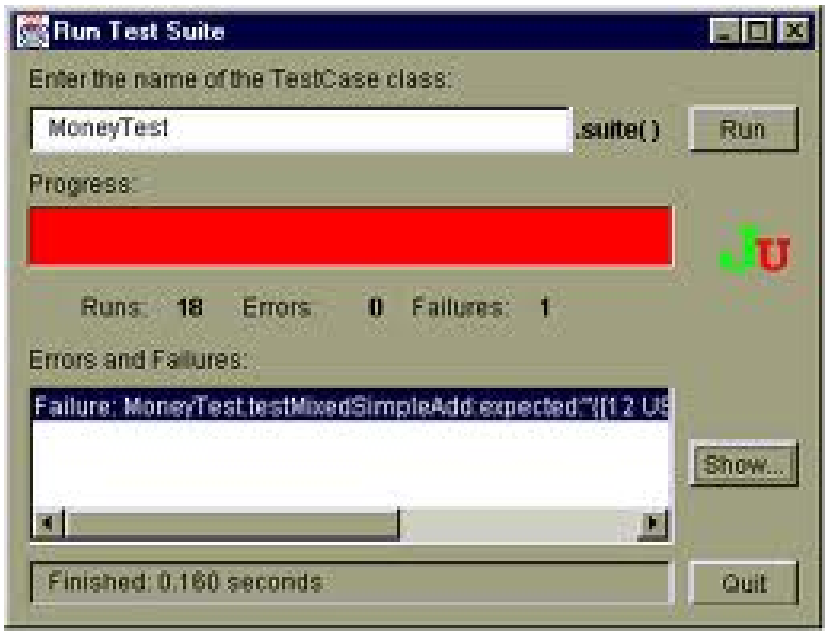
- Provide infrastructure to radically simplify:
  - Creating test routines (Test cases)
  - Running collections of tests (Test suites)
  - Summarizing results
- Key feature is collection of assert methods
  - Used to express expected results

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

- Generally specific to programming language (xUnit)
  - Java (JUnit)
  - Pnython (pyUnit)
  - C++ (cxxUnit, cppUnit)
  - Fortran (FRUIT, FUNIT, **pFUnit**)

GUI - JUnit in Eclipse





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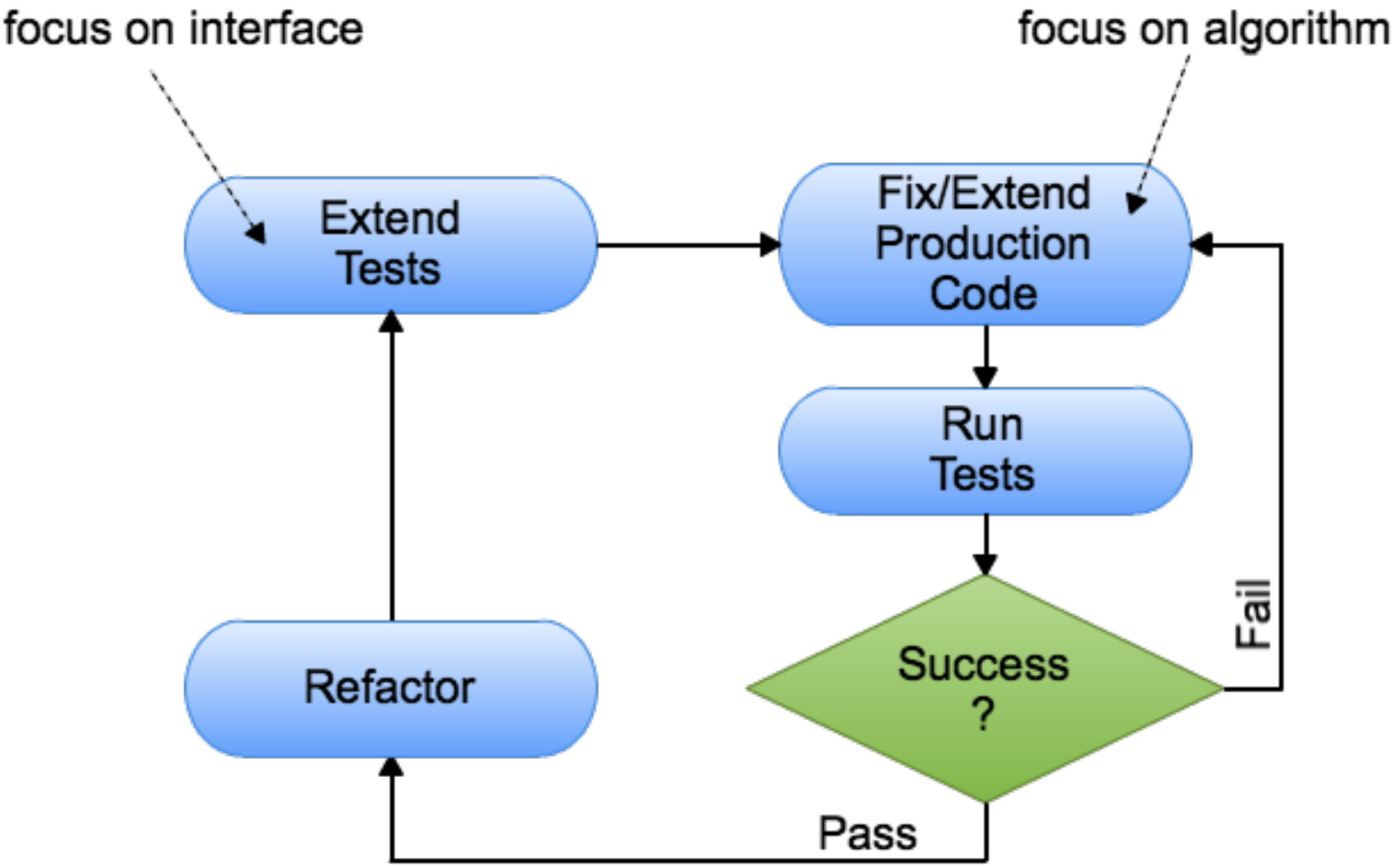
New paradigm

- 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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- **Quality implementation?**

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General mitigation strategy:

- Fine-grained implementation (each routine does just one thing)
- Test layers in isolation

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- Best case - usually asymtotic form with unknown leading coefficient!

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Conclusion: Decomposition and synthetic inputs yield testing tolerances that are of the same order as machine epsilon.

Test layers in isolation

Example: Procedure that does too much

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a = <complex expression>
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Higher level test ensures proper coupling, but not fully expanded arithmetic.

Test layers in isolation (cont'd)

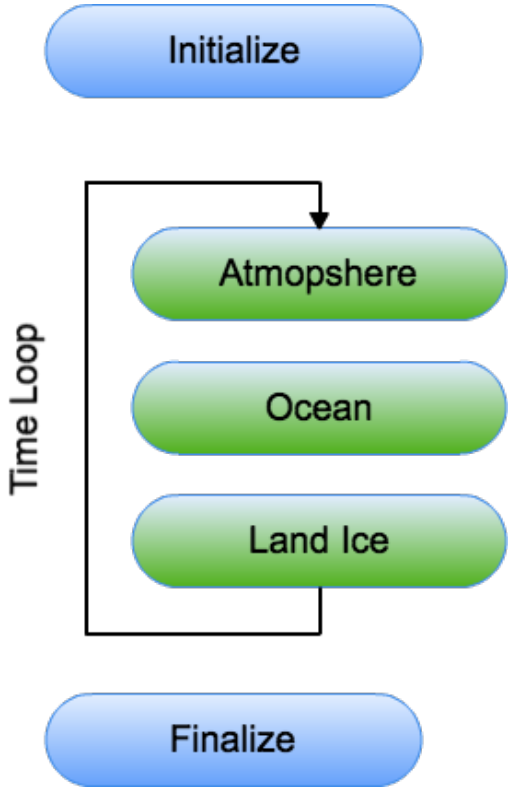
Consider the main loop of a climate model:

Do test

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

Do NOT test

- Calculations inside components



Much easier to do in practice with *objects* than with procedures.

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Consider Newton's three-body problem - no analytic solution

- Test generation of pairwise forces
- Test time integration (e.g., RK4)
- Use special cases that have solutions as additional tests

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  - Actual model *couples* layers - huge complexity

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- At the very least, TDD can reduce the frequency at which long integrations are needed/performed

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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

TDD and the legacy burden

- TDD was created for developing *new* code, and does not directly speak to maintaining legacy code.
- Adding 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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