Test Driven Development of Scientific Models

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Outline

The Tightrope Act

Software development should not feel like this

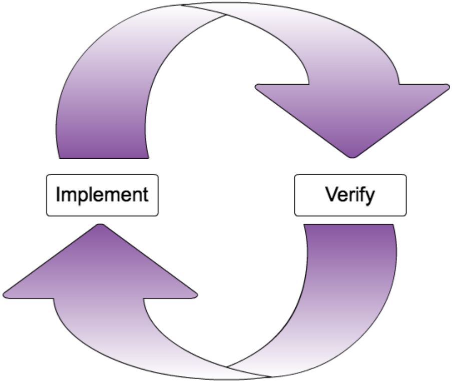
The Tightrope Act

... or even like this

The Tightrope Act

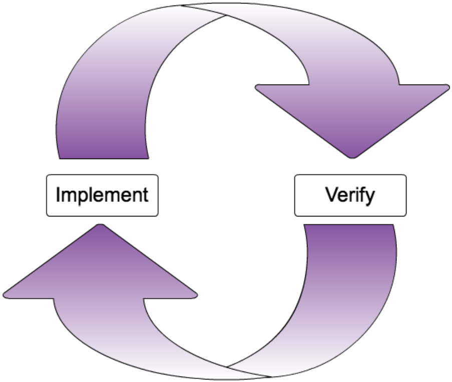
Hopefully something more like this

The Development Cycle



The Development Cycle

- **Extend**



The Development Cycle

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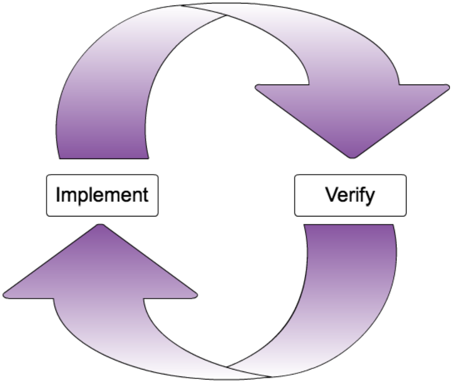
- **Fix**



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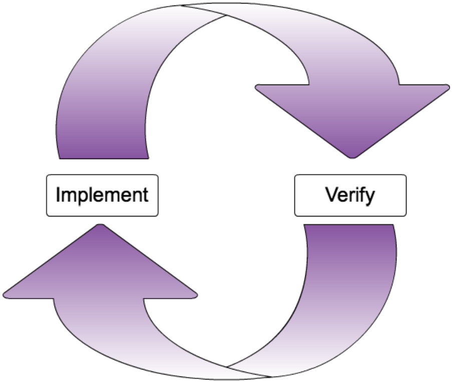
- **Port**



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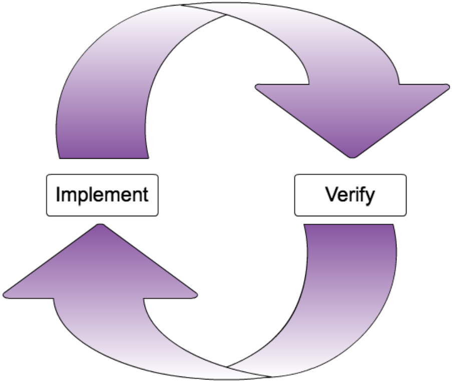

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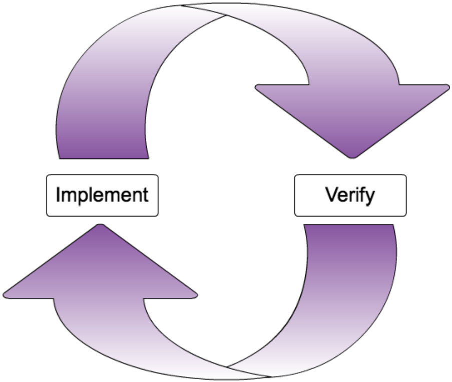

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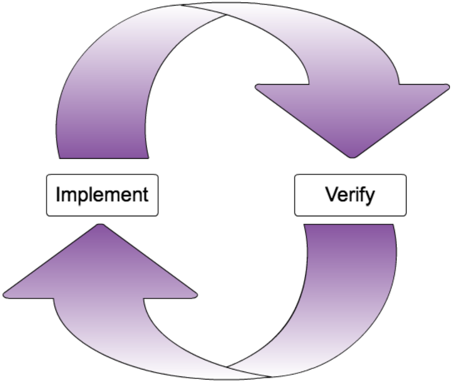

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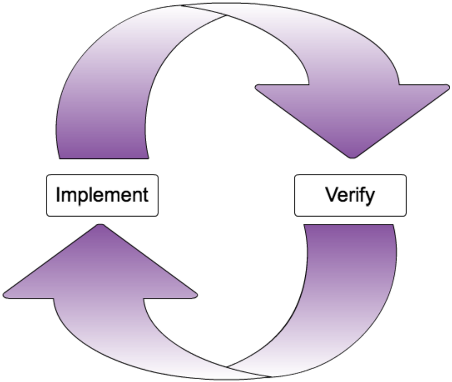

- Compiles?
- Executes?
- Looks ok?
- **Correct?**

Natural Time Scales

- Design
- Edit source
- Compilation
- Batch
  waiting in queue
- Execution
- Analysis

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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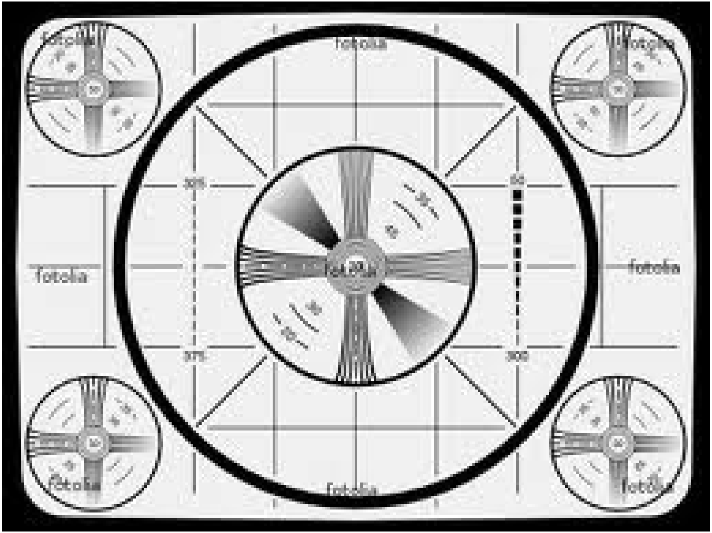
Testing



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- Localizes defects
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- **Decreases risk from change**

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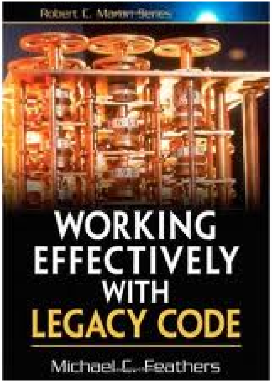
Michael Feathers
Working Effectively with Legacy Code



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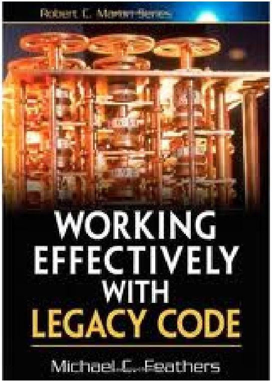

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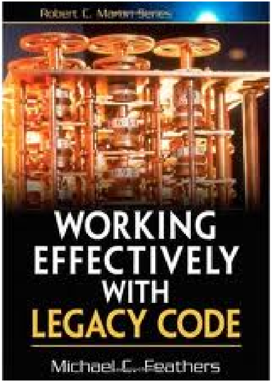

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This is also a barrier to involving pure software engineers in the development of our models.

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http://java.dzone.com/articles/unit-test-excuses

- James Sugrue

Just what is a test anyway?

Tests can exist in many forms

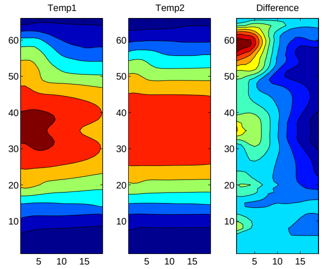
- Conditional termination:

```
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



Analogy with Scientific Method?

Reality	$\longrightarrow$	Requirements
Constraints: theory and data	$\longrightarrow$	Constraints: tests
Formulate hypothesis	$\longrightarrow$	Trial implementation
Perform experiment	$\longrightarrow$	Run tests
Refine hypothesis	$\longrightarrow$	Refine implementation

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- Clear intent

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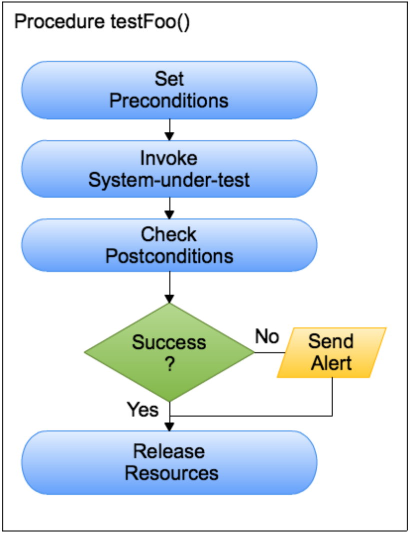

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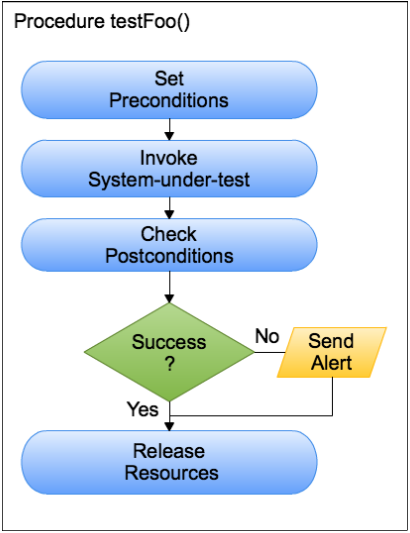

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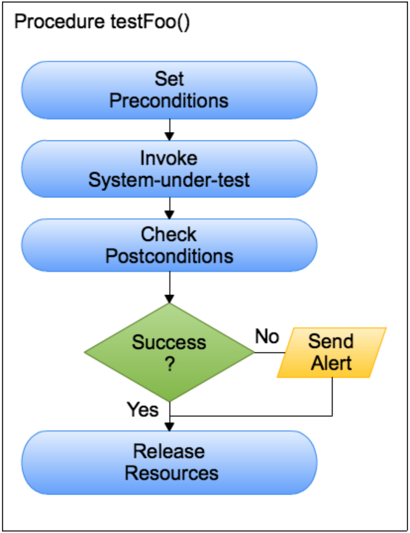

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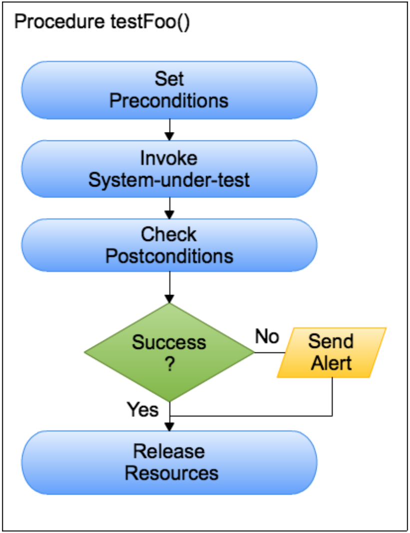

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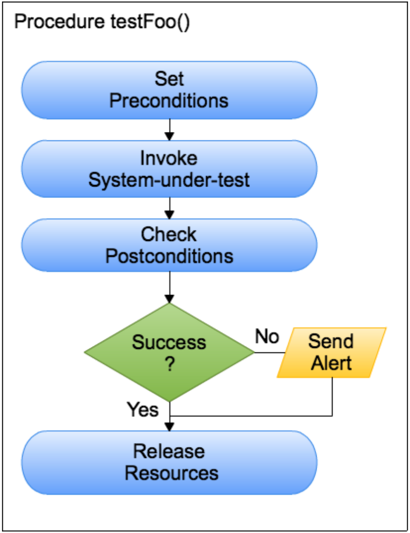

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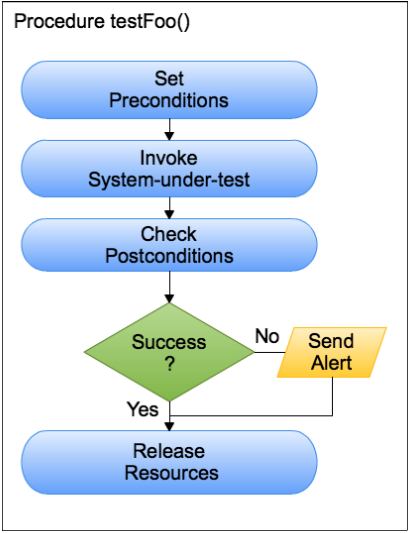

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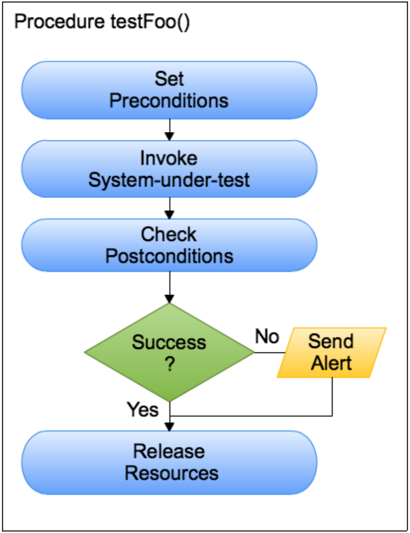

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Outline

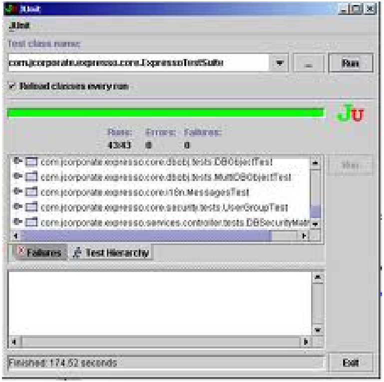
Testing Frameworks

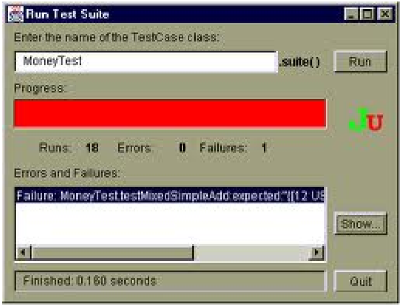
- Provide infrastructure to radically simplify:
  - Creating test routines (Test cases)
  - Running collections of tests (Test suites)
  - Summarizing results
- Key feature is collection of assert methods
  - Used to express expected results

```
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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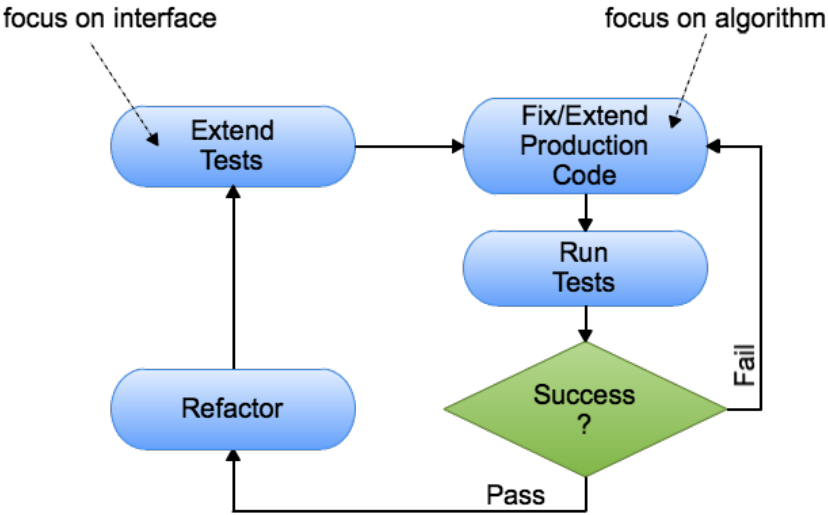
New paradigm

- 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?**

Anecdotal Testimony

- Many professional SEs are initially skeptical
  - High percentage refuse to go back to the old way after only a few days of exposure.
- Some projects drop bug tracking as unnecessary
- Often difficult to sell to management
  - "What? More lines of code?"

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    - But isnt the alternative is even worse?!!

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Software Testing vs Science/Validation

Software tests should only check *implementation*.

- Only a subset tests will express external requirements (i.e. implementation independent)
- Other tests will reflect implementation choices
- Use "convenient" input values - **not** *realistic* values

Consider tests for an ODE integrator implemented with RK4

- A generic test may be for a constant flow field - any integrator should get an "exact" answer
- A RK4 specific test may provide an artificial "flow field" that returns the values 1.,2.,3.,4. on subsequent calls *independent* of the coordinates

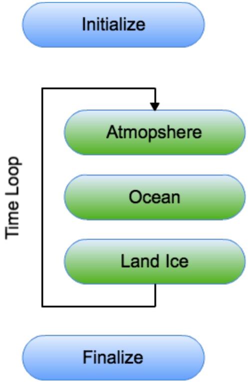
Test by Layers

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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- And of those, usually we just have an asymtotic form with unknown leading coefficient!

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Conclusion: If we write software as a composition of distinct small functions and subroutines, the errors can be reasonably bounded at each stage

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- If long integration gets incorrect results:
  1. Software defect: missing test
  2. Genuine science challenge
- TDD can reduce the frequency at which long integrations are needed/performed

TDD and Lack of Analytic Results

- Keep in mind: "How can you implement it if you cannot say what it should do?"
- Split into pieces - often each step has analytic solution
- Choose input values that are convenient

Consider a trivial case:

```
call assertEqual(3.14159265, areaOfCircle(1.))
call assertEqual(6.28..., areaOfCircle(2.))
```

What if instead the areaOfCircle() function accepted 2 arguments: "π" and r.

```
call assertEqual(1., areaOfCircle(1., 1.))
call assertEqual(4., areaOfCircle(1., 2.))
call assertEqual(2., areaOfCircle(2., 1.))
```

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- Long answer: Well, they shouldn't be ...
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  - Each layer of algorithm is tested separately
  - Layers of the production code are *coupled* - huge complexity

TDD and irreducible complexity

- Are the tests as complex as the implementation?
- Short answer: **No**
- Long answer: Well, they shouldn't be ...
  - Unit tests use specific inputs - implementation handles generic case
  - Each layer of algorithm is tested separately
  - Layers of the production code are *coupled* - huge complexity
  - Tests are *decoupled* - low complexity

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

TDD Best Practices

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- Small steps - each iteration $\ll$ 10 minutes

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TDD Best Practices

- Small steps - each iteration $\ll$ 10 minutes
- Small, readable tests
- Extremely fast execution - 1 ms/test or less
- *Ruthless* refactoring
- Verify that each test initially **fails**

TDD and Performance

- Optimized algorithms may require many steps within a single procedure
- TDD emphasizes small simple procedures
- Such an approach may lead to slow execution
- Solution: Bootstrapping
  - Use initial solution as unit test for optimized solution
  - Maintain *both* implementations

Experience to date

TDD has been used heavily within several projects at NASA

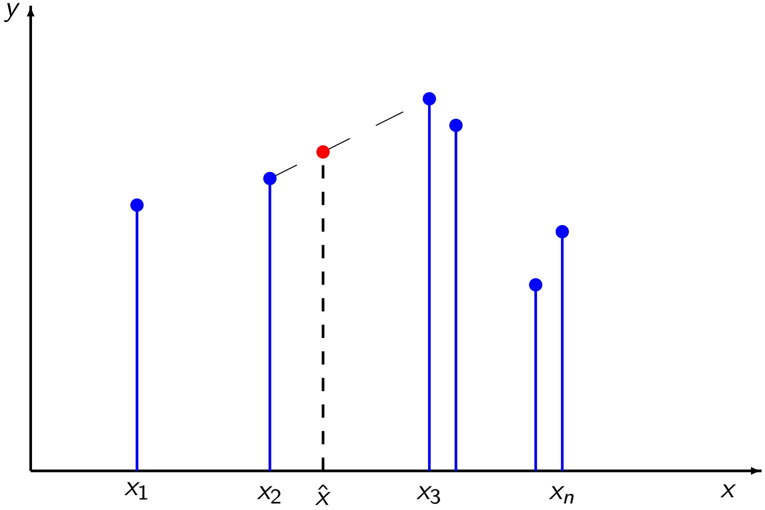
- Mostly for "infrastructure" portions - relatively little numerical alg.
- pFUnit
- DYNAMO - spectral MHD code on shperical shell
- GTRAJ - offline trajectory integration (C++)
- Snowfake - virtual snowfakes; Multi-lattice Snowfake

Observations:

- $\sim$ 1:1 ratio of test code to source code
- Works very well for *infrastructure*
- Learning curve
  - 1-2 days for technique
  - Weeks-months to wean old habits
  - Full benefit may require some sophistication

Outline

Linear Interpolation



Potential Tests

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- Computing node weights:

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\begin{aligned}
w_a &= \frac{x_{i+1} - \hat{x}}{x_{i+1} - x_i} \\
w_b &= 1 - w_a
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w_b &= 1 - w_a
\end{aligned}
$$

- Compute weighted sum: $\hat{y} = w_a f(x_i) + w_b f(x_{i+1})$

Bracketing Tests

```
index = bracket(nodes, x)
```

Case	Preconditions		Postcondition
	nodes	x	return

Bracketing Tests

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```

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	nodes	x	return
interior	$\{x\} = \{1, 2, 3\}$	$\hat{x} = 1.5$	$i = 1$

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other interior	$\{x\} = \{1, 2, 3\}$	$\hat{x} = 2.5$	$i = 2$

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at node	$\{x\} = \{1, 2, 3\}$	$\hat{x} = 2.0$	$i = 2$ (?)

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at node	$\{x\} = \{1, 2, 3\}$	$\hat{x} = 2.0$	$i = 2$ (?)
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at edge	$\{x\} = \{1, 2, 3\}$	$\hat{x} = 1.0$	$i = 1$ (?)
other edge	$\{x\} = \{1, 2, 3\}$	$\hat{x} = 3.0$	$i = 2$ (????)

Bracketing Tests

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index = bracket(nodes, x)
```

Case	**Preconditions** nodes	x	**Postcondition** return
interior	$\{x\} = \{1, 2, 3\}$	$\hat{x} = 1.5$	$i = 1$
other interior	$\{x\} = \{1, 2, 3\}$	$\hat{x} = 2.5$	$i = 2$
at node	$\{x\} = \{1, 2, 3\}$	$\hat{x} = 2.0$	$i = 2$ (?)
at edge	$\{x\} = \{1, 2, 3\}$	$\hat{x} = 1.0$	$i = 1$ (?)
other edge	$\{x\} = \{1, 2, 3\}$	$\hat{x} = 3.0$	$i = 2$ (????)
out-of-bounds	$\{x\} = \{1, 2, 3\}$	$\hat{x} = 1.5$	out-of-bounds error

Bracketing Tests

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index = bracket(nodes, x)
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Case	**Preconditions**		**Postcondition**
	nodes	x	return
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at node	$\{x\} = \{1, 2, 3\}$	$\hat{x} = 2.0$	$i = 2$ (?)
at edge	$\{x\} = \{1, 2, 3\}$	$\hat{x} = 1.0$	$i = 1$ (?)
other edge	$\{x\} = \{1, 2, 3\}$	$\hat{x} = 3.0$	$i = 2$ (????)
out-of-bounds	$\{x\} = \{1, 2, 3\}$	$\hat{x} = 1.5$	out-of-bounds error
out-of-order	$\{x\} = \{1, 2, 3\}$	$\hat{x} = 1.5$	out-of-order error

Example: Bracketing Test 1

- Preconditions: $\{x\} = \{1, 2, 3\}, \hat{x} = 1.5$
- Postcondition: return 1

Example: Bracketing Test 1

- Preconditions: $\{x\} = \{1, 2, 3\}, \hat{x} = 1.5$
- Postcondition: return 1

```
subroutine testBracket1()
   nodes = [1.,2.,3.]
   index = getBracket(nodes, 1.5)
   call assertEqual(1, index)
end subroutine
```

Example: Bracketing Test 1

- Preconditions: $\{x\} = \{1, 2, 3\}, \hat{x} = 1.5$
- Postcondition: return 1

```
subroutine testBracket1()
   call assertEqual(1, getBracket([1.,2.,3.], 1.5))
end subroutine
```

Example: Bracketing Test 1

- Preconditions: $\{x\} = \{1, 2, 3\}, \hat{x} = 1.5$
- Postcondition: return 1

```
subroutine testBracket1()
   call assertEqual(1, getBracket([1.,2.,3.], 1.5))
end subroutine
```

```
function getBracket(nodes, x) result(index)
   index = 1
end function
```

Example: Bracketing Test 2

- Preconditions: $\{x\} = \{1, 2, 3\}, \hat{x} = 2.5$
- Postcondition: return 2

```
subroutine testBracket2()
   nodes = [1.,2.,3.]
   index = getBracket(nodes, 2.5)
   call assertEqual(2, index)
end subroutine
```

Example: Bracketing Test 2

- Preconditions: $\{x\} = \{1, 2, 3\}, \hat{x} = 2.5$
- Postcondition: return 2

```
subroutine testBracket2()
   nodes = [1.,2.,3.]
   index = getBracket(nodes, 2.5)
   call assertEqual(2, index)
end subroutine
```

```
function getBracket(nodes, x) result(index)
   if (x > nodes(2)) then
      index = 2
   else
      index = 1
   end if
end function
```

Example: Bracketing Test 2

- Preconditions: $\{x\} = \{1, 2, 3\}, \hat{x} = 2.5$
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```
subroutine testBracket2()
   nodes = [1.,2.,3.]
   index = getBracket(nodes, 2.5)
   call assertEqual(2, index)
end subroutine
```

```
function getBracket(nodes, x) result(index)
   if (x > nodes(2)) then
      index = 2
   else
      index = 1
   end if
end function
```

Generalize ...

Example: Bracketing Test 2

- Preconditions: $\{x\} = \{1, 2, 3\}, \hat{x} = 2.5$
- Postcondition: return 2

```
subroutine testBracket2()
  nodes = [1.,2.,3.]
  index = getBracket(nodes, 2.5)
  call assertEqual(2, index)
end subroutine
```

```
function getBracket(nodes, x) result(index)

  do i = 1, size(nodes)     1
    if (nodes(i+1) > x) index = i
  end do

end function
```

Tests for Computing Weights

```
index = bracket(nodes, x)
```

Case	**Preconditions**		**Postcondition**
	interval	x	weights

Tests for Computing Weights

```
index = bracket(nodes, x)
```

Case	Preconditions		Postcondition
	interval	x	weights
lower bound	$[1., 2.]$	$\hat{x} = 1.0$	$w = [1.0, 0.0]$

Tests for Computing Weights

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Case	**Preconditions**		**Postcondition**
	interval	x	weights
lower bound	$[1., 2.]$	$\hat{x} = 1.0$	$w = [1.0, 0.0]$
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Tests for Computing Weights

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Case	**Preconditions**		**Postcondition**
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interior	$[1., 2.]$	$\hat{x} = 1.5$	$w = [0.5, 0.5]$

Tests for Computing Weights

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    index = bracket(nodes, x)
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	interval	x	weights
lower bound	$[1., 2.]$	$\hat{x} = 1.0$	$w = [1.0, 0.0]$
upper bound	$[1., 2.]$	$\hat{x} = 1.0$	$w = [0.0, 1.0]$
interior	$[1., 2.]$	$\hat{x} = 1.5$	$w = [0.5, 0.5]$
big interval slope	$[1., 3.]$	$\hat{x} = 1.5$	$w = [0.75, 0.25]$

Tests for Computing Weights

```
index = bracket(nodes, x)
```

Case	**Preconditions**		**Postcondition**
	interval	x	weights
lower bound	$[1., 2.]$	$\hat{x} = 1.0$	$w = [1.0, 0.0]$
upper bound	$[1., 2.]$	$\hat{x} = 1.0$	$w = [0.0, 1.0]$
interior	$[1., 2.]$	$\hat{x} = 1.5$	$w = [0.5, 0.5]$
big interval slope	$[1., 3.]$	$\hat{x} = 1.5$	$w = [0.75, 0.25]$
degenerate	$[1., 1.]$	$\hat{x} = 1.0$	degenerate error

Tests for Computing Weights

```
    index = bracket(nodes, x)
```

Case	Preconditions		Postcondition
	interval	x	weights
lower bound	$[1., 2.]$	$\hat{x} = 1.0$	$w = [1.0, 0.0]$
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degenerate	$[1., 1.]$	$\hat{x} = 1.0$	degenerate error
out-of-bounds	$[1., 2.]$	$\hat{x} = 0.5$	out-of-bounds error

Example: Weights Test 1

- Precondition: $[a, b] = [1., 2.], \hat{x} = 1.0$
- Postcondition: $w = \{1.0, 0.0\}$

```
subroutine testWeight1()
   real :: interval(2), weights(2)
   real :: x
   interval = [1.,2.]
   weights = computeWeights(interval, 1.0)
   call assertEqual([1.0,0.0], weights)
end subroutine testWeight1
```

```
real function computeWeights(interval, x) result(weights)
   real, intent(in) :: interval(2)
   real, intent(in) :: x
   weights = [1.0,0.0]
end function
```

Example: Tying it together

- Precondition:
  - $\{(x,y)_i\} = \{(1,1),(2,1),(4,1)\}$
  - $\hat{x} = 3$
- Postcondition: $\hat{y} = 1$.

```
subroutine testInterpolateConstantY()
   real :: nodes(2,3)
   nodes = reshape([[1,1],[2,1],[4,1]], shape=[2,3])
   call assertEqual(1.0, interpolate(nodes, 3.0))
end subroutine testInterpolate1
```

```
function interpolate(nodes, x)
   real, intent(in) :: nodes(:,:)
   y = 1
end function interpolate
```

Example: Tying it together

- Precondition:
  - $\{(x, y)_i\} = \{(1, 1), (2, 3), (4, 1)\}$
  - $\hat{x} = 3$
- Postcondition: $\hat{y} = 2$.

```
subroutine testInterpolate1()
   real :: nodes(2,3)
   nodes = reshape([[1,1],[2,3],[4,1]], shape=[2,3])
   call assertEqual(1.0, interpolate(nodes, 3.0))
end subroutine testInterpolate1
```

```
function interpolate(nodes, x) result(y)
   integer :: i
   real :: weights(2), xAtEndPoints(2), yAtEndpoints(2)

   i = getBracket(nodes(1,:), x)

   xAtEndPoints = nodes(1,i)   ! used derived type?
   yAtEndpoints = nodes(2,i)
   weights = computeWeights(nodes(1,[i,i+1]), x)

   y = sum(weights * yAtEndpoints)
end function interpolate
```

Outline

pFUnit - Fortran Unit testing framework

- Tests written in Fortran
- Supports testing of parallel (MPI) algorithms
- Support for multi-dimensional array assertions
- Written in standard F95 (plus a tiny bit of F2003)
- Developed using TDD

Tutorial in the afternoon sessioon

References

- pFUnit: http://sourceforge.net/projects/pfunit/
- Tutorial materials
  - https://modelingguru.nasa.gov/docs/DOC-1982
  - https://modelingguru.nasa.gov/docs/DOC-1983
  - https://modelingguru.nasa.gov/docs/DOC-1984
- TDD Blog https://modelingguru.nasa.gov/blogs/modelingwithtdd
- *Test-Driven Development: By Example* - Kent Beck
- Mller and Padberg,"About the Return on Investment of Test-Driven Development," http://www.ipd.uka.de/mitarbeiter/muellerm/publications/edser03.pdf
- *Refactoring: Improving the Design of Existing Code* - Martin Fowler
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- These slides https://modelingguru.nasa.gov/docs/DOC-2222