Managing Defects in HPC Software Development

Presented to
Argonne Training Program on Extreme-Scale Computing (ATPESC)

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NNSA National Nuclear Security Administration
U.S. DEPARTMENT OF ENERGY | Office of Science

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- If you require sparkly things in the presentation to keep you awake, please refer back to item (1).

Outline

Research and HPC Code

Challenge

Manage SQE with discovery

Posit

Consider a new algorithm implemented in a multidimensional, parallel code.

- Theory predicts second-order convergence.
- Computational results are first-order instead of second-order.
- Is this a code bug or an error in analysis?

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Research and HPC Code

- In other words, SQE and methods research are not only compatible, they are essential
- This is especially true for parallel scientific software, which is much more difficult to design, test, and analyze than serial software.
- We are interested in this case in performing software verification
- Software verification is a method for removing defects at code construction time

What is SQE

- SQE is the practice of managing the cost and quality of a software product
- **Guiding Principle**
  The cost of defect resolution increases with time from defect introduction*
- **Things fall apart**
  - Defects in model development
  - Defects in algorithmic selection
  - Defects in requirements
  - Defects in implementation

How to mitigate defects

- There are many methods for defect management
- Three techniques we use for software verification in an HPC environment
  - The complete development lifecycle
  - Unit-testing
  - Design-by-Contract©
- This list is by no means exhaustive (or a complete SQE process)
  - Notably missing, **reviews**
  - We do them, they work, but I'm not here to talk about them
- However, taken together these can help catch defects before they become an unbearable expense

Requirements Management in Scientific Software

- Requirements can be very difficult to pin down in scientific software development:
  - the vector keeps changing as new things are learned
  - as a community we often know what we want, but aren't necessarily good at saying it
- Software verification helps disambiguate language-based requirements into functional specifications
- As requirements change, software verification helps ensure that the software is keeping pace.
- Agility is key in scientific software development:
  - rapid prototyping
  - testing new methods, algorithms, and features

Complete Development Lifecycle

- The developer is reponsible for the **complete** implementation of a feature including:
  - Requirements
  - Derivation
  - Construction
  - Deployment
- Documentation and verification is implicit in each phase
- Reviews and team collaboration are essential

Developers are responsible for all phases of code development

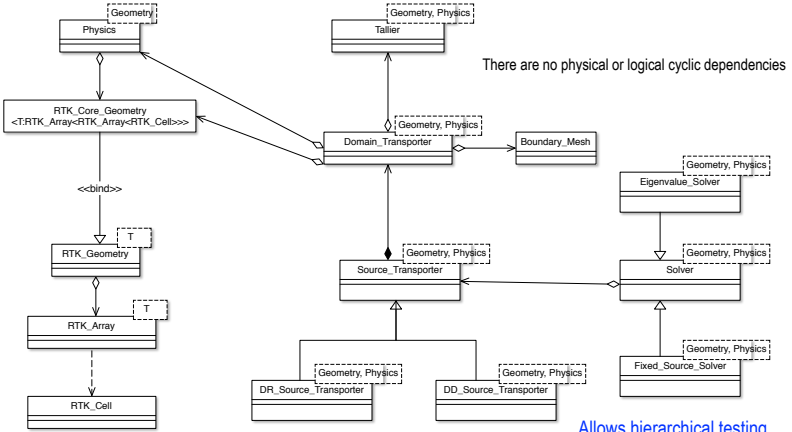
Unit Testing

Unit testing is a form of software verification

- It ensures that each part of the software performs its contracted task
- The effectiveness of unit-testing is greatly enhanced by the following two code design practices:
  - Acyclic code design
  - Design-by-Contract© (see later)

We practice a method of unit testing in which the unit test is written either before, or concurrently with, the executable code.

Acyclic Code Design



An Example—Reactor Geometry

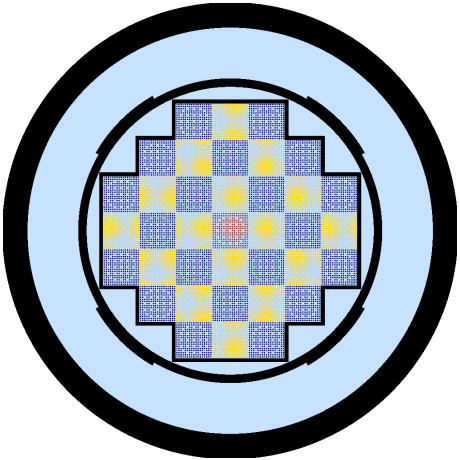


Figure: Small modular reactor core model.

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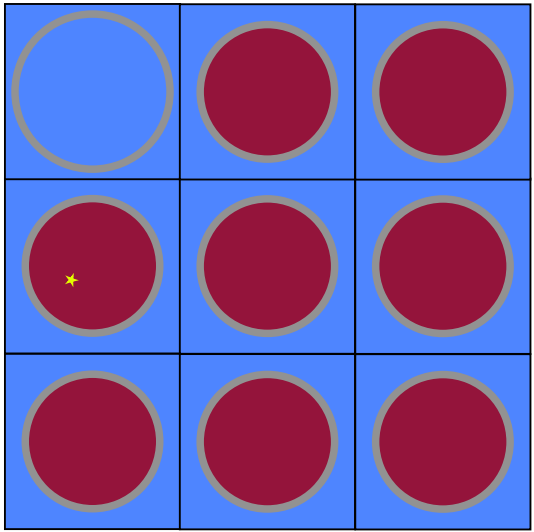

1. Sample starting neutron

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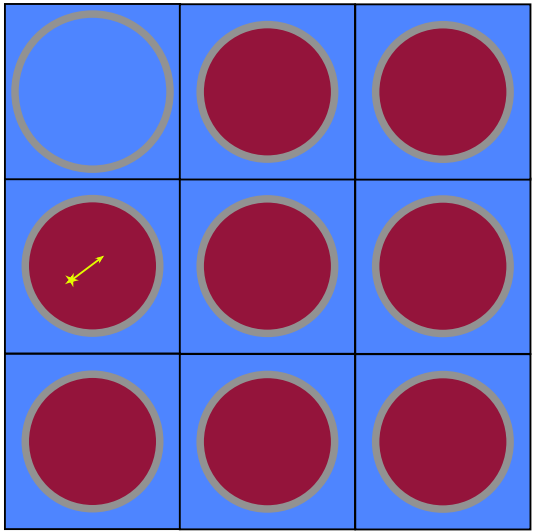

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$$d_{\text{col}} = \frac{\log(\xi)}{\sigma(\mathbf{r}, E)}$$

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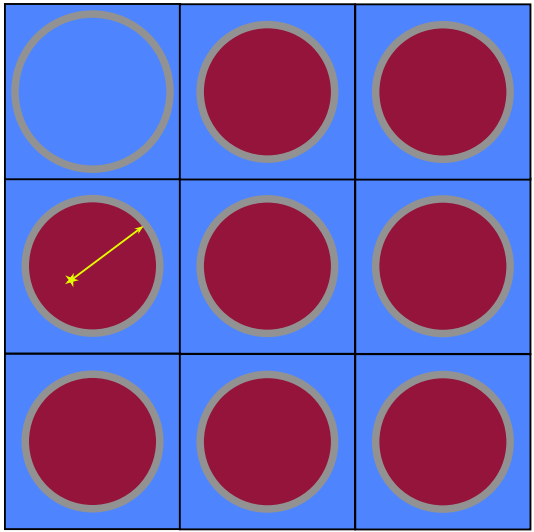

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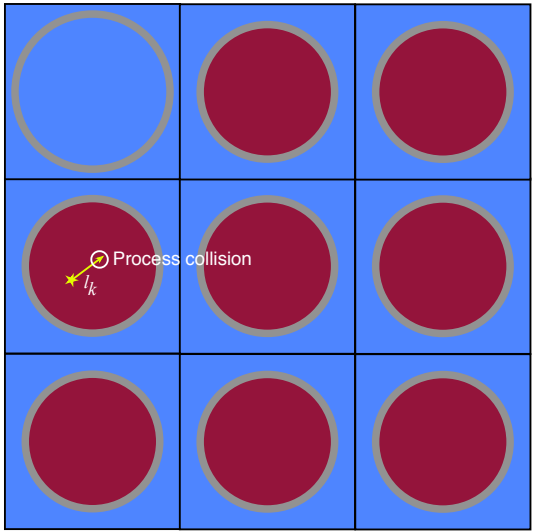

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3. Calculate distance to boundary
4. Move particle
5. Tally state data

$$\phi = \frac{1}{V} \sum_k l_k$$

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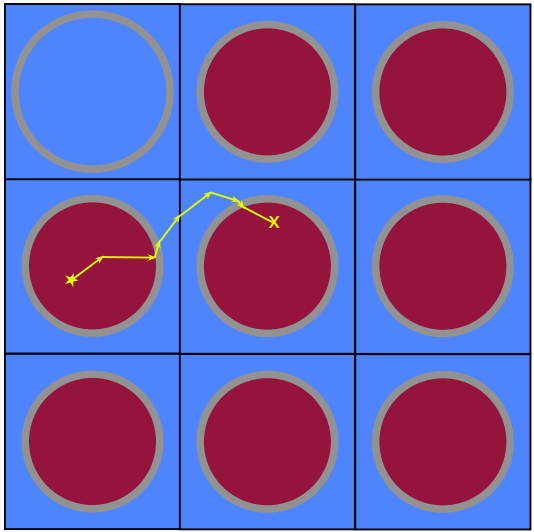

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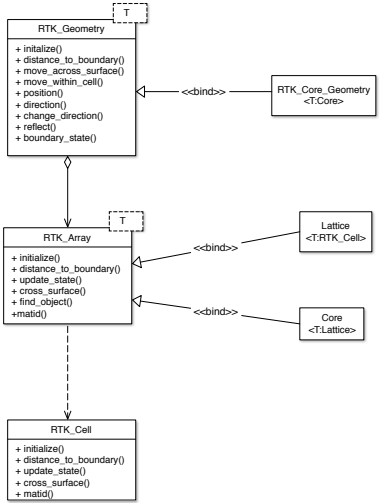
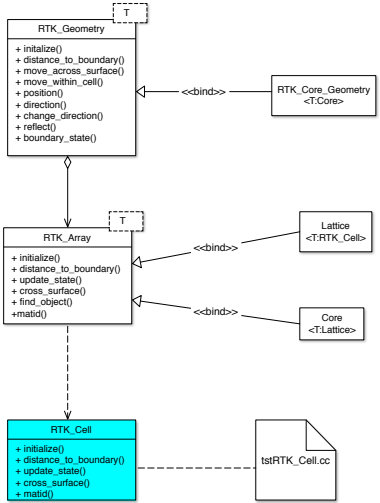
6. Repeat 2–5

First Level—RTK_Cell



- Here is the class diagram for the `RTK_Geometry` part of the code

First Level—RTK_Cell



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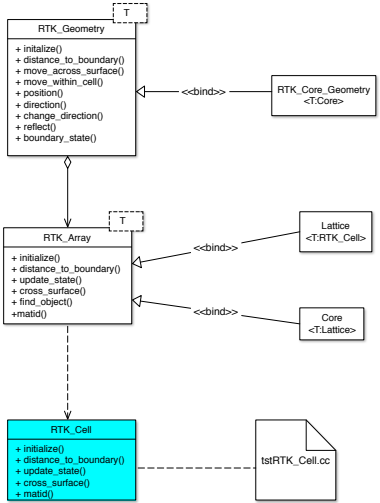


- Here is the class diagram for the `RTK_Geometry` part of the code
- Starting at the lowest level of the class hierarchy, we can write a unit test that unambiguously tests `RTK_Cell`
- There are many frameworks that support this—**GoogleTest**, TeuchosTest (Trilinos)
- Some extra details are required to support advanced architectures

tstRTK_Cell.cc—The old way

```
#include "Nemesis/gtest/nemesis_gtest.hh"

TEST(SingleShell, track)
{
    RTK_Cell pin1(1, 0.54, 10, 1.26, 14.28);

    pin1.initialize(Vector(0.0, 0.55, 0.0), state);
    EXPECT_EQ(1, state.region);
    EXPECT_EQ(0, state.segment);
    EXPECT_EQ(1, pin1.cell(state.region, state.segment));

    Vector r     = Vector(0.0, 0.59, 0.0);
    Vector omega = Vector(1.0, 0.0, 0.0);
    pin1.initialize(r, state);
    pin1.distance_to_boundary(r, omega, state);
    EXPECT_SOFTEQ(state.dist_to_next_region, 0.63, 1.e-12);
    EXPECT_EQ(Geo_State::PLUS_X, state.exiting_face);
    EXPECT_EQ(1, state.region);

    // ...
}
```

- In MP/multithreaded codes this way straitforward
- Instantiate the object and test its state and behavior
- “garbage-in/garbage-out”
- “Hand” calculations stored in repository using Jupyter Notebook
- On heterogeneous computing environments extra work is required

tstRTK_Cell.cc—The “new” way

```
#include "Nemesis/gtest/nemesis_gtest.hh"
#include "RTK_Cell_Tester.hh"

TEST_F(Single_Shell, construction)
{
    construct();
}

TEST_F(Single_Shell, tracking)
{
    track();
}
```

Host-side driver—host-only test code and defined tests

RTK_Cell_Tester.hh

```
#include "Nemesis/gtest/Gtest_Functions.hh"
#include "Geometria/rtk/RTK_Cell.hh"

class Single_Shell : public Base
{
  protected:

    void SetUp()
    {
        SP_Cell pin1 = std::make_shared<RTK_Cell>(1, 0.54, 10, 1.26, 14.28);
        SP_Cell pin2 = std::make_shared<RTK_Cell>(1, 0.45, 2, 1.2, 14.28);
        pins         = {pin1, pin2};
    }

    void construct();
    void track();

    Vec_Cell pins;
};
```

Bridge code—connects host-side driver with kernel implementation

RTK_Cell_Tester.cu

```
void Single_Shell::track()
{
    geometria_cuda::RTK_Cell_DMM dmm(*pins[1]);
    auto pin = dmm.device_instance();

    thrust::device_vector<int>    ints(50, -1);
    thrust::device_vector<double> dbls(50, -1);

    single_shell_kernel2<<<1,1>>>(
        pin, ints.data().get(), dbls.data().get());

    thrust::host_vector<int>    rints(ints.begin(),
                                      ints.end());
    thrust::host_vector<double> rdbls(dbls.begin(),
                                      dbls.end());

    int    n   = 0, m = 0;
    double eps = 1.0e-6;

    EXPECT_EQ(1, rints[n++]);
    EXPECT_SOFTEQ(rdbls[m++], 1.2334036420, eps);
    EXPECT_EQ(State::INTERNAL, rints[n++]);
    EXPECT_EQ(0, rints[n++]);

    // ...
```

```
__global__
void single_shell_kernel2(
    geometria_cuda::RTK_Cell  pin,
    int                       *ints,
    double                    *dbls)
{
    State  state;
    Vector r, omega;
    int    n = 0, m = 0;

    // Pin intersection tests
    {
        r     = {  0.43,   0.51,   1.20};
        omega = { -0.07450781,  -0.17272265,   0.98214840};
        pin.initialize(r, state);
        ints[n++] = state.region;
        pin.distance_to_boundary(r, omega, state);
        ints[n++] = state.exiting_face;
        ints[n++] = state.next_region;
        dbls[m++] = state.dist_to_next_region;
    }

    // ...
```

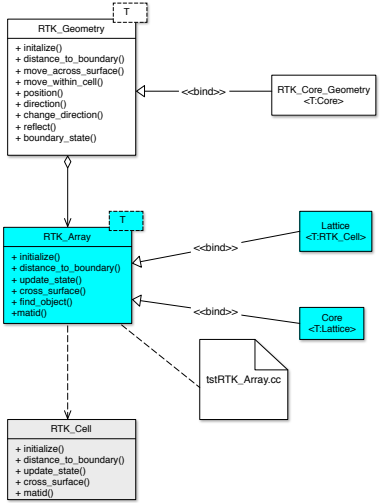
Test Output

```
Testing on 1 processors
Exnihilo 6.2 (branch 'omnibus_cuda' #20e8c851 on 2017JUL10) [debug] [DBC=7]
SCALE 6.3 (r23123: #c743536b on 2017JUL06) [debug] [DBC=7]
[==========] Running 2 tests from 1 test case.
[----------] Global test environment set-up.
[----------] 2 tests from Single_Shell
[ RUN      ] Single_Shell.construction
[       OK ] Single_Shell.construction (381 ms)
[ RUN      ] Single_Shell.tracking
[       OK ] Single_Shell.tracking (2 ms)
[----------] 2 tests from Single_Shell (383 ms total)

[----------] Global test environment tear-down
[==========] 2 tests from 1 test case ran. (384 ms total)
[  PASSED  ] 2 tests.
In ./GeometriaCUDA_tstRTK_Cell.exe, overall test result: PASSED
```

```
PACKAGE_ADD_CUDA_LIBRARY(
  Geometria_cuda_test_cuda
  SOURCES RTK_Array_Tester.cu
  DEPLIBS Geometria_cuda
  TESTONLY)

ADD_NEMESIS_TEST(tstRTK_Cell.cc  NP 1
  DEPLIBS Geometria_cuda_test_cuda)
```

- Integrated into CMake build system
- Compile-Edit-Debug development cycle
- Continuous integration

Second Level—RTK_Array



- Having verified `RTK_Cell` we proceed to the next level
- Individual unit-tests work their way up dependency chain
- After completion of a feature, unit tests remain in the code base for both regression and continuous integration testing

Design-by-Contract©

- DBC enforces a function “contract” by testing the input, execution, and output of a function.
- In other words, DBC provides a software mechanism for enforcing a design contract on a function.
- DBC is also known as Programming by Contract and Contract First Development.
- See Meyer, Bertrand: Design by Contract, in *Advances in Object-Oriented Software Engineering*, eds. D. Mandrioli and B. Meyer, Prentice Hall, 1991, pp. 1-50 for more details.

DBC Implementation

- Some languages (Eiffel, GNU C^2) have built in support for DBC.
- DBC is implemented in our codes using M4 (FORTRAN) or CPP (C/C++).
- Types in C++ or FORTRAN modules are automatically checked by the compiler:
  - `Require`: input conditions
  - `Check`: execution conditions
  - `Ensure`: output conditions
- DBC macros can be toggled at compile time to avoid performance costs associated with in-code tests.
- We also support device implementations

A DBC Example

- You are asked to provide a routine to calculate square roots—ok this is a manufactured example
- Being a clever person you realize you can solve this as a nonlinear problem using Newton's method:

$$x_{n+1} = x_n + \frac{f(x_n)}{f'(x_n)},$$

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where $f(x_n) = x_n^2 - S$

- You deliver your unit-tested, verified solution:

```
double my_sqrt(double S)
{
    double xn = 1.0;

    for (int n = 0; n < 10; ++n)
    {
        xn = 0.5 * (xn + S / xn);
    }

    return xn;
}
```

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- You reply that the routine was thoroughly tested and is performing as designed, so what gives
- Pandemonium ensues

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- Nothing is more common in scientific programming
- How could DBC have helped?
- Lets look at how adding DBC may have aided things

This is a defect resulting from ambigous requirements

- Nothing is more common in scientific programming
- How could DBC have helped?
- Lets look at how adding DBC may have aided things
- First, we decide we will not handle complex math
- Second, we check for a tolerance at the end

```
double my_sqrt(double S)
{
    Require(S > 0.0);

    double xn = 1.0;

    for (int n = 0; n < 10; ++n)
    {
        xn = 0.5 * (xn + S / xn);
    }

    Ensure(std::fabs(xn*xn - S) > 1.0e-6 * S)
    return xn;
}
```

Moral of the story

- This still won't win any programmer-of-the-year awards, but you get the point
- Adding DBC "contracts" allows both developers and clients to codify potentially ambiguous requirements
- In particular, at review time DBC can help a reviewer determine if the requested service is doing what is required
- Downstream, if the function is used in manner that is outside of design parameters, at least we know

Real DBC Example—`distance_to_boundary`

```
__device__
void RTK_Cell::distance_to_boundary(
    const Space_Vector &r,
    const Space_Vector &omega,
    Geo_State_t        &state) const
{
    DEVICE_REQUIRE(soft_equiv(vector_magnitude(omega), 1., 1.e-6));
    DEVICE_REQUIRE(omega[X]<0.0          ?
                   r[X] >= d_extent[X][LO] :
                   r[X] <= d_extent[X][HI]);
    DEVICE_REQUIRE(omega[Y]<0.0          ?
                   r[Y] >= d_extent[Y][LO] :
                   r[Y] <= d_extent[Y][HI]);
    DEVICE_REQUIRE(omega[Z]<0.0 ?
                   r[Z] >= 0.0  :
                   r[Z] <= d_z);
    // ...
    DEVICE_CHECK(db >= 0.0);
    // ...

    DEVICE_ENSURE(state.dist_to_next_region >= 0.0);
    DEVICE_ENSURE(state.exiting_face == Geo_State_t::INTERNAL ?
                  state.next_region >= 0 : true);
    DEVICE_ENSURE(state.next_segment >= 0 && state.next_segment < d_segments);
```

- Valid argument types are checked by the compiler
- `DEVICE_REQUIRE` checks that input arguments are and object is in a valid state
- `DEVICE_CHECK` in-function checks
- `DEVICE_ENSURE` object and arguments are in a valid state at output

Software Verification Advantages

The purpose of unit-testing is to provide software verification as close to code construction time as possible.

- finds code defects at construction time
- provides an automated, explicit review of the code and enables Continuous Integration
  - a mechanism for review is to have one developer write the test and the primary developer writes the code
  - when the test passes, the software component is automatically reviewed
  - provides a testing basis for Continuous Integration

Software Verification Advantages

- makes porting to new platforms easier
- easier to find esoteric compile/link-time errors
- DBC can be used to verify interfaces to client code
- DBC incurs no cost in production code
- easier to run profiling, memory, and development tools on unit tests than on a full executable
- unambiguous statement of code design requirements

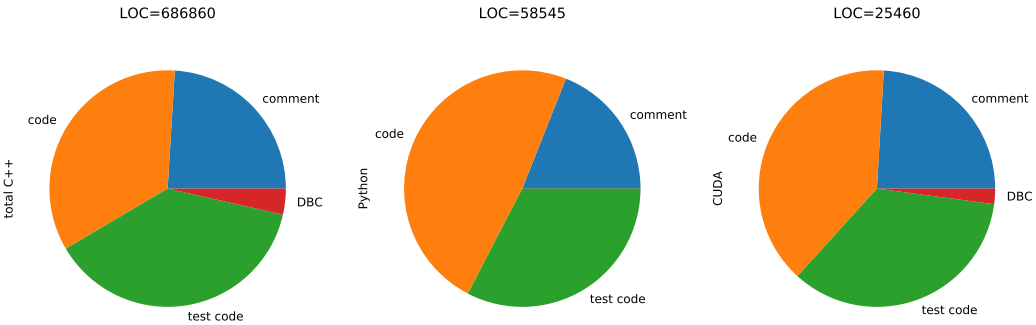
Software Verification Advantages

- provides a sanity check on code refactors
- incorporating timing data allows a time-history profile of code performance to be compiled:
  - run automated unit-tests nightly
  - as new code is developed compare timing histories to catch inefficient or costly implementations
- provides simplified “usage” documentation for a piece of code
  - in our example, a new developer could easily learn the mechanics of the `RTK_Geometry` component by studying the unit tests

Disadvantages and Costs

- The most significant disadvantage is the perceived cost associated with unit tests
- Our experience shows a cost of between 4-8 to 1 in writing code with unit tests
- This cost is minimal compared to the debugging cost incurred throughout a product lifecycle
- In other words, the disadvantages are few unless you have developers who unfailingly write “Bug-Free Code”
- Codes that are not structured according to acyclic design concepts may have prohibitive unit-test costs
- Finding and abiding the 80/20 rule takes developer experience

Yes, we actually do this



Final Thoughts

- Review one takeaway: The cost of defect resolution increases with time from defect introduction
- Use this as a guiding principle to improve productivity and tailor it to fit your needs—you don't need to do what we or others do!
- Applying this principle will sometimes add up-front costs, but it has the advantage of catching defects when they are introduced; this will result in significant savings downstream

Acknowledgments

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