Disclaimer

This talk comes in two parts, a general philosophy part and a case study part

- The general part applies to many (all?) long-running scientific software projects
- The solutions from our case study may or may not apply to your project; they’re meant as examples
Outline

• Problems faced by long-lived scientific codes
• LANL’s experience in the xRage code project
• Recommendations for other projects
Long-lived scientific codes

• Discussions of best software practices sometimes assume (implicitly?) that you’re starting a new project and a new code

• But what if you have an ongoing, years- or decades-old project?
  – Large, pre-existing code base
  – Existing code team with established habits
  – Significant user base, already using the code regularly

• Often such projects have major challenges to software quality
  – Complex, hastily-written code
  – Incomplete testing
  – Inadequate documentation
  – Little or no software process
  – A culture that says, “Why should we do all this fancy process stuff? We’re getting along fine without it!”
What do you mean by “getting along fine”?  

• Historically, it has usually meant that the code:  
  – Has the capabilities the users want  
  – And has them ASAP  

• This approach can be successful in the short term...  
  – Can build up a user base  
  – Can meet deliverables, produce papers, get grants renewed, etc.  

• ...but it has problems that show up in the longer term  
  – Code is written hastily, hard to understand  
  – Design is ad-hoc  
  – Difficult for code team to maintain, extend  
  – Difficult for new team members to learn  
  – Difficult to optimize for new architectures  

• In other words, it’s not sustainable
What do you mean by “getting along fine”? (2)

- A modern, better definition would be that the code:
  - Is understandable, maintainable
  - Is extensible
  - Is well-tested
  - Is well-documented
  - Is portable to modern architectures
  - And still has the capabilities the users want
  - And has them (reasonably) quickly

- This is more sustainable for the long term
Changing practices requires changing values and culture

- A project decides what it values, and grows a culture that reflects those values.
- This affects many aspects of a code project:
  - Languages, programming models, tools used (or not used)
  - Staffing (how many developers? what background?)
  - Training, career development
  - Performance evaluations
  - Tasking, scheduling, deliverables
- These all reinforce each other, push the project in a certain direction.
- It’s very hard to change that direction without (at least partly) changing values and culture.
Changing practices can require changing code

- Sometimes best practices and modern tools have built-in assumptions that older codes don’t satisfy:
  - Unit testing assumes self-contained units
  - Shared ownership of code assumes understandable code that any developer can reason about
  - And so on...

- Result: changing practices may have to go hand-in-hand with changing code
  - This may make starting the process harder
  - But once it does start, it can become a “virtuous cycle”

So what does it look like to put all this into practice?
Case study: The LANL xRage code

- xRage is an Eulerian AMR radiation-hydrodynamics code
- Original code written ~1990
- Has been used successfully in several application areas
- Contains about 470K lines of source code
  - Not counting numerous third-party libraries, from LANL and elsewhere
- Mostly Fortran 90, some C/C++
- MPI-only parallelism

xRage applications:
asteroid impact simulations, shape charge experiments, Inertial Confinement Fusion simulations
The need for modernizing xRage

20+ years of high-pressure work left xRage with significant technical debt. This made it difficult to:
• understand the code flow or data flow
• maintain the code
• add new features
• train new developers as older staff retire
• refactor for advanced architectures, such as Trinity, Sierra, . . .

These factors (especially the last two) made us realize that things needed to change!
Prerequisite #1: Management support for culture change

Management saw the need for doing things differently, was willing to make changes:

- Added a CS co-lead to the project
- Shifted project resources to support more CS/SE staff
- Allocated part of domain scientists’ time to modernization work
- Scaled back development of new physics features, milestone commitments
Prerequisite #2: Regression test suite

- Before: We had a regression test suite, but it wasn’t well-maintained
- As refactoring started: team committed to keeping tests passing (“wall of green”)
- At first, all tests were integrated tests
  - Unit tests were added later
- Nightly, weekly test runs are automated, results emailed to team
- Tests serve as a safety net as we refactor
What to tackle first?

Several possible tasks:
- Move to modern build system (e.g. CMake)?
- Implement unit testing?
- Clean up our tangled dependency structure?

We decided to do cleanup first
- Cleaner code has immediate benefit
- Can’t do unit tests on a hairball code
- Could use CMake on a hairball code, but that’s not what CMake is designed for

xRage dependency graph, 2014-10-01
(the “hairball” graph)
Untangling dependencies

• Any file could use data, call routines from any other file
• Our strategy to change this:
  – Change existing code base in place
  – Separate code into packages of related functionality with well-defined interfaces
  – Move toward a cleaner, simpler design
• Some techniques:
  – Create derived types for package state, pass through argument lists
  – Find misplaced code and move it to a proper place
  – Lift some function calls (e.g., coupling) to higher-level packages
  – Deprecate/remove unneeded calls
Untangling dependencies (2)

After about 15 months of work, this process led to a much simpler graph (right)

- Graph is levelized, has no cycles!
- Interfaces between packages are better-defined
- This makes it easier to understand, reason about the code
- This enables other changes on a per-package basis
  - Unit testing, documentation
  - Code cleanup
  - Performance optimization
  - Physics improvements

xRage dependency graph, 2016-01-11
Where we are now

Task list:

- Levelize dependency graph (complete)
- Refactor build system to use libraries, enforce levelization (complete)
- Add unit tests (infrastructure complete, test writing ongoing)
- Document packages (ongoing)
- Clean up code within packages (ongoing)
- Work on performance optimization (ongoing)
- Move from home-grown build system to CMake (prototyped)
- Move from SVN version control to Git/Gitlab (planning)
- Set up Gitlab-CI continuous integration (planning)
Some recommendations to other projects

• Get management support for culture change - this is crucial!
• Use regression tests as a safety net as you refactor
• Resist the temptation to move to a shiny new tool just because it’s shiny and new
  – Prioritize tasks/changes by value added to the project
• Find the right balance between code/process improvement and user support
  – Both are important!
Resources

General resources:

  - Specific mechanisms are now outdated, but...
  - General principles still apply to all languages, not just C++

- Feathers, *Working Effectively with Legacy Code*

More details on xRage refactoring:

- Ferenbaugh et al., *Modernizing a Long-Lived Production Physics Code*, SC16 poster
  
Resources (2)

Tools we’ve found useful for xRage:

- **Understand** static visual analysis tool
  
  http://scitools.com

- **Graphviz** graph visualization for dependency graphs
  
  http://graphviz.org

- **pFUnit** unit test framework for Fortran
  
  http://pfunit.sourceforge.net

- **Google Test** unit test framework for C/C++
  
  https://github.com/google/googletest
Questions?

Thanks for your attention!

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