Bringing Best Practices to a Long-Lived Production Code

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HPC Best Practices Webinar
January 17, 2018

Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA

LA-UR-18-20135

Disclaimer

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

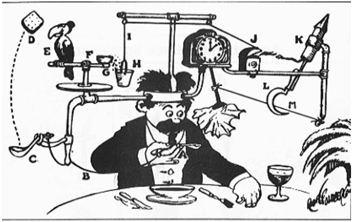
- The general part applies to many (all?) long-running scientific software projects
- The solutions from our case study may or may not apply to your project; they're meant as examples

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

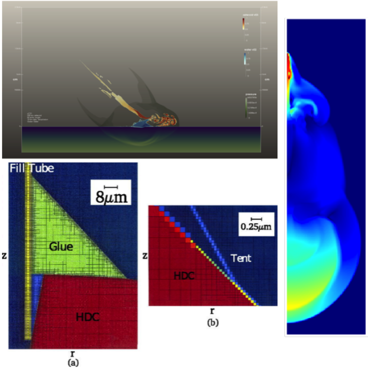
Changing practices can require changing code

- 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

Collaborative Test System

Los Alamos National Laboratory Collaborative Test System

APPLIED PHYSICS DIVISION

CRESTONE Project
Tue Jul 26 07:00:43 MDT 2016

CROSS PLATFORM RESULTS (Nobel)			
	CI	ML	TR
	intel	intel	intel
	default	openmpi	default
	xrage	xrage	xrage
Totals	147/147	147/147	146/146
RunTime	13234	15270	6725
Test			
AMR_dart	Pass 239	Pass 189	Pass 109
AMR_dblast	Pass 187	Pass 235	Pass 111
AMR_sod	Pass 26	Pass 66	Pass 18
AnisoFailStretch	Pass 74	Pass 410	Pass 81
Cond	Pass 12	Pass 22	Pass 9
CrushAlum	Pass 99	Pass 110	Pass 56
CuAirRP	Pass 76	Pass 48	Pass 36
Exact_Cond1dLin	Pass 8	Pass 10	Pass 5
Exact_Cond2dLin	Pass 138	Pass 105	Pass 57
Exact_Cond2dNl	Pass 140	Pass 101	Pass 58
HE_AR	Pass 70	Pass 109	Pass 41
HE_CerroGrande	Pass 35	Pass 35	Pass 21
HE_FF	Pass 11	Pass 12	Pass 8
HE_FFPB	Pass 237	Pass 182	Pass 113
HE_FF_RS	Pass 23	Pass 35	Pass 18
HE_IG	Pass 22	Pass 28	Pass 15
HE_PB	Pass 15	Pass 30	Pass 13
HE_SURF	Pass 231	Pass 245	Pass 121
HE_SURFmerge	Pass 13	Pass 15	Pass 10
HE_SURFplus	Pass 203	Pass 191	Pass 110
HE_SURFplusZND	Pass 48	Pass 33	Pass 32

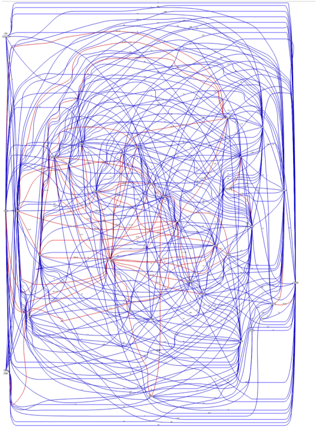
What to tackle first?

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

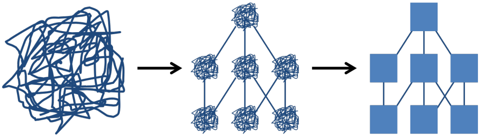
- Cleaner code has immediate benefit
- Can't do unit tests on a hairball code
- *Could* use CMake on a hairball code, but that's not what CMake is designed for



xRage dependency graph, 2014-10-01 (the "hairball" graph)

Untangling dependencies

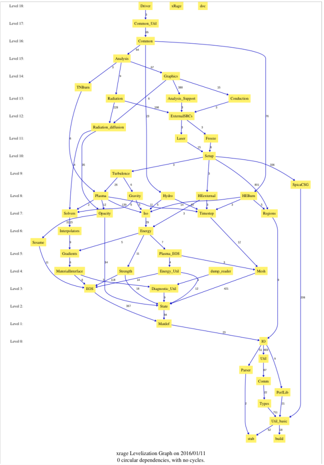
- Any file could use data, call routines from any other file
- Our strategy to change this:
  - Change existing code base *in place*
  - Separate code into *packages* of related functionality with well-defined interfaces
  - Move toward a cleaner, simpler design
- Some techniques:
  - Create derived 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:

- Lakos, *Large-Scale C++ Software Design* (1996)
  - 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
  `http://sc16.supercomputing.org/sc-archive/tech_poster/tech_poster_pages/post196.html`

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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