

The State of Trilinos Software Engineering

Recent Progress, Current Status, and Future Issues

Roscoe A. Bartlett

http://www.cs.sandia.gov/~rabartl/

Department of Optimization & Uncertainty Quantification Trilinos Software Engineering Technologies and Integration Lead

Sandia National Laboratories

Trilinos Users Group Meeting 2010, Nov. 4, 2010



Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.



Part I

The Software Engineering Challenge in Computational Science & Engineering

and

The Role that Trilinos Can Play



Factors Driving Increased Complexity in CSE Software

Progress in Computational Science & Engineering (CSE) is occurring primarily through the creation of greater varieties of increasingly more complex algorithms and methods

- o **Discretization**: a) geometry, b) meshing, b) approximation, c) adaptive refinement, ...
- Parallelization: a) parallel support, b) load balancing, ...
- General numerics: a) automatic differentiation, ...
- Solvers: a) linear-algebra, b) linear solvers, c) preconditioners, d) nonlinear solvers, e) time integration, ...
- Analysis capabilities: a) embedded error-estimation, b) embedded sensitivities, c) stability analysis and bifurcation, d) embedded optimization, d) embedded UQ, ...
- Input/Output ...
- Visualization ...
- o ...

Complexity is also increasing due to new computer architectures (exascale):

Multi-core CPUs and GPUs => More complex programming and software architecture

- Decreased "mean time to failure" => More complex "robust" algorithms
- Each technology requires specialized PhD-level expertise to implement
- Almost all technologies can be exploited to solve the full problem (i.e. design, V&V, UQ, ...)
- o Set of algorithms/software is too large for any single organization to create

These treads will lead to greater than an order-of-magnitude increase in CSE software complexity which will require an order-of-magnitude increase in knowledge/skills/dedication/discipline in software design/integration/engineering!



The CSE Software Engineering Challenge

- Develop a confederation of trusted, high-quality, reusable, compatible, software packages/components including capabilities for:
 - o Discretization: a) geometry, b) meshing, b) approximation, c) adaptive refinement, ...
 - **Parallelization**: a) parallel support, b) load balancing, ...
 - o General numerics: a) automatic differentiation, ...
 - Solvers: a) linear-algebra, b) linear solvers, c) preconditioners, d) nonlinear solvers,
 e) time integration, ...
 - Analysis capabilities: a) embedded error-estimation, b) embedded sensitivities, c) stability analysis and bifurcation, d) embedded optimization, d) embedded UQ, ...
 - o Input/Output ...
 - Visualization ...
 - o ...



Trilinos itself is a smaller example of this!





Many CSE organizations and individuals are adverse to using externally developed CSE software!

Using externally developed software can be as risk!

- External software can be hard to learn
- External software may not do what you need
- Upgrades of external software can be risky:
 - Breaks in backward compatibility?
 - Regressions in capability?
- External software may not be well supported
- External software may not be support over long term (e.g. KAI C++, CCA)

What can reduce the risk of depending on external software?

- Apply strong software engineering processes and practices (high quality, low defects, frequent releases, regulated backward compatibility, ...)
- Ideally ... Provide long term commitment and support (i.e. 10-30 years)
- Minimally ... Develop Self-Sustaining Software (open source, clear intent, clean design, extremely well tested, minimal dependencies, sufficient documentation, ...)



Requirements/Challenges for a Confederation of CSE Codes

 Software quality and usability 	Rol
 Design, testing, training, standards, collaborative development (Agile tech practices) 	• F
 Building the software in a consistent way and linking 	р
=> Common build approach (e.g. CMake)	• [
 Reusability and interoperability of software components 	а
=> Incremental Agile design, runtime resource management,	р
 Critical new functionality development 	C
=> Closer development and integration models	• (
 Upgrading compatible versions of software 	ir
=> Frequent fixed-time releases, regulated backward compatibility	E H
 Safe upgrades of software 	C
=> Regulated backward compatibility, reducing defects	
 Documentation, tutorials, user comprehension 	• (
=> SE education, better documentation and examples	n
• Self-sustaining software (open source, clean design, clean implementation, well tested with unit tests and system verification tests, minimal dependencies, barely sufficient documentation,)	

=> Anyone can maintain it!

- Long term maintenance and support
 - = > Stable organizations, stable projects, stable staff

Role of Trilinos?

- R&D in SE practices for CSE?
- Demonstrate and advocate good SE practices in SE community?
- Coordinate and interact (lead) efforts in the CSE community?
- Collect more and more CSE software?





PART II

Recent Progress and Current Status of Trilinos Software Engineering





Recent Progress in Trilinos SE Infrastructure

- Moved to Git version control system
 - More flexible development models
 - □ More stable code repository
- □ SIERRA Trilinos Almost Continuous Integration process:
 - Nightly testing (< 48 hour delay) of a lot of Trilinos (Teuchos through MOOCHO) on many platforms (GCC, Intel, AIX, Pathscale, PGI, etc.)
 - □ SIERRA takes snapshots of Trilinos for releases
- Greater Trilinos development stability:
 - □ Allow for daily integration testing and daily updating of customer APPs
- □ Support for deprecated warnings for GCC with macros
- □ Improvement in release processes (see Jim's talk later):
 - □ More frequent releases => lead to less instability of releases
- External repositories and add-on Trilinos packages (see later slide)
 - Partitioning of copyrighted and non-copyrighted packages
 - □ Scalable non-direct growth (LIMEExt, TerminalPackages, Panzer, etc.)
 - Allow users to extend Trilinos with add-on packages
- □ Testing improvements (see later slide):
 - □ Introduction of CATEGORIES keyword (e.g. BASIC, NIGHTLY, etc.)
 - Better pre-push and post-push CI testing
 - □ Faster test computers (Teuchos+ 32 min on 12 core Linux/AMD for \$7K)
- More extensive/safer Teuchos memory management classes (see later slide) s



Example:

- \$ cd \$TRILINOS_HOME_DIR
- \$ eg clone software.sandia.gov:/space/git/preCopyrightTrilinos
- \$ cd \$BUILD_DIR
- \$./do-configure -DTrilinos_EXTRA_REPOSITORIES=preCopyrightTrilinos \
 -DTrilinos_ENABLE_Amesos2 ...

After that, all of the extra packages defined in <EXTRAREPO> will appear in the list of official Trilinos packages and you are free to enable any that you would like just like any other Trilinos package.

For more details see:

\$TRILINOS_HOME_DIR/cmake/TrilinosCMakeQuickstart.txt
\$TRILINOS_HOME_DIR/cmake/HOWTO.ADD_EXTRA_REPO





Teuchos C++ Memory Management Classes/Idioms

SANDIA REPORT

2010-2234 Unlimited Release Printed June 2010

Teuchos C++ Memory Management Classes, Idioms, and Related Topics

The Complete Reference

A Comprehensive Strategy for Safe and Efficient Memory Management

in C++ for High Performance Computing

Roscoe Bartlett

Prepared by Sandia National Laboratories Abuquerque, New Mexico 87185 and Livermore, California 94550

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- The solution to eliminating undefined behavior in C++
- Eliminate direct use of raw
- Family of collaborating classes: RCP, Ptr, ArrayView, ArrayRCP, Array, Tuple
- Extremely good debug-mode runtime checking and feedback.
- Raw-pointer performance in nondebug build.
- Circular references not automatically handled
- Great debug-mode runtime support for catching and diagnosing circular references and tools to resolve them
- Not trivial to learn classes/idioms
- Static analysis tool feedback would help a lot!





PART III

Immediate Needs in Trilinos Software Engineering





Immediate needs and Related Efforts in Trilinos SE

- Generalize and externalize the Trilinos CMake/CTest/CDash system
 - □ Allow other projects to fully exploit the Trilinos SE infrastructure
 - □ Will be used by projects like NEAMS, CASL and perhaps others
- □ Centralize information and keep up to date on Trilinos websites (see Jim's talk)
 - Do Google site searches first to answer questions!!!!!!
 - □ Example: "cmake version site:software.sandia.gov/trilinos/developer/"
- □ Further needed improvements in Trilinos release-related efforts and processes
 - □ Automated tarball testing
 - Automated installation testing
 - □ Move (almost) all release-related work **before** the branch
 - □ See Jim's talk ...
- □ Need more improvements to CDash server robustness
 - □ Kitware to fix and/or new dedicated CDash server?
- □ Need more effort/discipline in maintaining Trilinos testing processes
- □ Improvements in Testing (see slide)
- □ Sub-Package Support (see slide)
- Need more Trilinos Framework Staff!





Testing Improvement Needs





Murphy's Law for Software:

"For any attribute you claim your software has, if you don't have strong automated tests to provide strong evidence for that property, you can almost guarantee that the property will not exist just when it will do the most damage."

Example:

Customer: "Your algorithm X does not scale very well"

Developer: "Nonsense, I tested the scalability myself just a few months ago"

Customer: "Did you test scalability on the exact release version I am using?"

Developer: "No, I did not have time to do the testing again."

Customer: "What could have changed?"

Developer: "Some code somewhere obviously or perhaps something else?"

Example of claims about software:

- "The software is efficient"
- "The software scales"
- "The software is well tested"
- "The software works"



Trilinos Testing Infrastructure and Needed Improvements Weekly Coverage Testing Nightly Regression Tests Secondary Stable (SS) Weekly Memory (Valgrind) Testing CATEGORIES [BASIC NIGHTLY] (more platforms, more TPLs) **Correctness Testing** Asynchronous CI Tests Performance Tests Secondary Stable (SS) Secondary Stable (SS) CATEGORIES [BASIC NIGHTLY] CATEGORIES PERFORMANCE (post-push CTest/Cdash, Linux/GCC) (CTest/CDash) Synchronous CI Tests Scalability Tests? Primary Stable (PS) Secondary Stable (SS) **CATEGORIES BASIC** CATEGORIES SCALING??? (pre-push (CTest/CDash) checkin-test.py)

Current status and needs for each testing category:

- Synchronous CI Tests: Better use of checkin-test.py script; need faster better (unit) tests
- Asynchronous CI Tests: Automatic, fast feedback (e.g. < 20 min); need better notifications
- □ Nightly Regression Tests: Linux/Mac, GCC/Intel; need better coverage and more platforms
- □ Weekly Coverage Tests: Has recurring upload failures
- □ Weekly Memory Tests: Not currently running; need a dedicated machine to run weekly
- □ Performance Testing: Just a few Teuchos tests (see TSDM10); need many more tests
- Scalability Tests: Not even defined, no CATEGORIES support yet, need Ctest/Cdash support



Automated Performance Testing Support in Trilinos

Always build the executable

PACKAGE_ADD_EXECUTABLE(RCP_PerformanceTests CATEGORIES BASIC PERFORMANCE COMM serial mpi SOURCES RCP_Performance_UnitTests.cpp

)

Correctness tests that always runs (fast)
PACKAGE_ADD_TEST(
 RCP_PerformanceTests
 CATEGORIES BASIC PERFORMANCE
 COMM serial mpi
 NUM_MPI_PROCS 1
 POSTFIX_AND_ARGS_0 base
 --show-test-details=ALL --max-array-size=100000
 STANDARD_PASS_OUTPUT
)

Properties of good performance tests

- Hard pass/fail based on (relative) time limits
- Make timings relative to a simple related calculation
 - Example: compare dot product in Tpetra compared to simple loops with raw arrays
- Allow fine-grained adjustment of relative timings for different machines
- Adjust the number of timing loops according to a "relative CPU speed"
 - Default relative CPU speed 1.0 is for a *very* slow machine
- Only enable and run performance tests in an optimized build on an unloaded machine
- Always build the performance test executables and test "correctness" of the test
- Have a simple fast "correctness" test as the default mode to run

Enabling performance tests

\$ cmake -DTrilinos_REL_CPU_SPEED=1e+3 \
 -DTrilinos_TEST_CATEGORY-PEFORMANCE ...



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• Nightly Performance Testing: (SERIAL_PERF build currently running nightly on godel)

```
SET(BUILD_DIR_NAME SERIAL_PERF)
SET(Trilinos_PACKAGES Teuchos)
```

```
SET( EXTRA_CONFIGURE_OPTIONS
```

"-DCMAKE_CXX_FLAGS:STRING=-O3\ -DBOOST_SP_DISABLE_THREADS"

```
"-DCMAKE_C_FLAGS:STRING=\"-03\""
```

```
"-DCMAKE_Fortran_FLAGS:STRING=\"-05\""
```

- "-DDART_TESTING_TIMEOUT:STRING=120"
- "-DTrilinos_TEST_CATEGORIES:STRING=PERFORMANCE"

```
"-DTrilinos_REL_CPU_SPEED:STRING=1e+3"
```

- •••
-)
- ToDos:
 - Add strong performance tests for a *lot* more code
 - Convert existing "weak" performance tests to be "strong" performance tests
 - Should there be a separate dashboard track for performance tests?
 - Add an MPI_PERF build? If done carefully, this can be useful.





Trilinos CMake Sub-Package Support





Existing package dependency logic can enable many more packages than is needed for sufficient testing

Example: Enable Tpetra

\$ checkin-test.py --enable-packages=Tpetra -configure

- Enabled packages (libraries) (28/52): Teuchos, RTOp, Kokkos, Epetra, Zoltan, Shards, Triutils, Tpetra, EpetraExt, Thyra, Isorropia, AztecOO, Galeri, Amesos, Pamgen, Ifpack, ML, Belos, Stratimikos, Meros, Anasazi, RBGen, Sacado, Intrepid, NOX, Rythmos, MOOCHO, Sundance
- Enabled packages (tests/examples) (10/52): Tpetra, Belos, Stratimikos, Anasazi, RBGen, NOX, Rythmos, MOOCHO, Sundance
- -> Problem: Stratimikos, Rythmos, MOOCHO, and Sundance don't execute one line of Tpetra code!
- General Problem: Current CMake build system does not respect the true dependency structure that exists in these packages.





Package Cohesion OO Principles:

- REP (Release-Reuse Equivalency Principle): The granule of reuse is the granule of release.
- CCP (Common Closure Principle): The classes in a package should be closed together against the same kinds of changes. A change that affects a closed package affects all the classes in that package and no other packages.
- CRP (Common Reuse Principle): The classes in a package are used together. If you reuse one of the classes in a package, you reuse them all.

Package Coupling OO Principles:

- ADP (Acyclic Dependencies Principle): Allow no cycles in the package dependency graph.
- SDP (Stable Dependencies Principle): Depend in the direction of stability.
- SAP (Stable Abstractions Principle): A package should be as abstract as it is stable.

Problem: Many Trilinos packages violate the SE packaging principles most importantly the CRP

Source: Martin, Robert C. Agile Software Development (Principles, Patterns, and Practices). Prentice Hall, 2003





CMake Sub-Package Architecture: The Idea



- Trilinos packages: More natural feature/social/user/documentation collections
- Trilinos sub-packages: Dependency-management SE packages (hidden from user)
- Speeds up pre-push rebuilds and testing with checkin-test.py tool
- Provided greater control over feature selection
- Helps to minimize superficial entangling dependencies
- Minimizes the number of top-level packages
- Hides complexity form the user
- However, some SE packages will still be needed due to dependency issues
- Git allows us to move files around into different directories so we can now do this!
- See Trilinos Framework Backlog Item 4644





PART IV

Longer Term Issues in Trilinos Software Engineering





Regulated Backward Compatibility





Example of the Need for Backward Compatibility



Multiple releases of Trilinos presents a possible problem with complex applications

Solution:

=> Provide sufficient backward compatibility of Trilinos X through Trilinos SIERRA Y+1





- Backward compatibility is critical for:
 - Safe upgrades of new releases
 - Composability and compatibility of different software collections
- Maintaining backward compatibility for all time has downsides:
 - Testing/proving backward compatibility is expensive and costly
 - Encourages not changing (refactoring) existing interfaces etc.
 - => Leads to software "entropy" which kills a software product
- A compromise: Regulated backward compatibility (Trilinos approach)
 - Maintain a window of "sufficient" backward compatibility over major version numbers (e.g. 1-2 years)
 - Provide "Deprecated" compiler warnings
 - Example: GCC's <u>deprecated</u> attribute enabled with -DTrilinos_SHOW_DEPRCATED_WARNINGS:BOOL=ON
 - Drop backward compatibility between major version numbers
 - [Future] Provide strong automated testing of Trilinos backward compatibility





- Trilinos Version Numbering X.Y.Z:
 - X: Defines backward compatibility set of releases
 - Y: Major release (off the master branch) number in backward compatible set
 - Z: Minor releases off the release branch X.Y
 - Y and Z: Even numbers = release, odd numbers = dev
 - Makes logic with Trilinos_version.h easier
- Backward comparability between releases:
 - Example: Trilinos10.6 is backward compatible with 10.0 through 10.4
 - Example: Trilinos 11.X is not compatible with Trilinos 10.Y



Example: Major Trilinos versions change every 2 years with 2 releases per year



Collaborative Development (e.g. Code Reviews)

and

Static Analysis Tools





Collaborative Development (e.g. Code Reviews)

- Importance of Collaborative Development Practices ("Code Complete 2nd")
 - Testing alone will only achieve the detection of 60% or less of defects (Jones 2000)
 - High-volume beta testing (> 1000 sites) achieves less than 85% defect detection.
 - Formal code reviews alone achieve 60% defect detection rates
 - Formal code reviews combined with testing can achieve 95% or higher defect detection/removal (Jones 200)
 - Per defect, reviews are 20 times cheaper than black-box testing (Freedman and Weinberg 1990).
 - You can't afford not to implement some type of code review process!
- Approaches to doing effective collaborative development ("Code Complete 2nd")
 - Formal code reviews
 - Inform reviews (e.g. code reading, walk-throughs, dog-and-pony shows, ...)
 - Pair programming
- From "Implementing Lean Software Development":
 - Issues that are well addressed by code reviews:
 - Readability, comprehensibility, change tolerance, duplicate code, design quality (good naming, good use of OO patterns and principles, etc.)
 - => catching requirements defects and design defects
 - Issues <u>not</u> well addressed by code reviews:
 - Catching low-level construction defects => Use TDD and unit testing instead
 - Enforcing low-level coding standards => Use static analysis tools instead

Integrated Static Analysis Tools in Development Envir

- Leaning and improving quality through automated tools and continuous feedback?
 - Example: Writing better C++ using g++ -Wall -pedantic -ansi ...
 - We don't expect everyone to be experts in C++ to write C++ code because modern C++ compilers provide lots of feedback and help in learning C++.
- Tools/analyses/feedback not integrated into development environment are ignored!
 - Example: What is the coverage of your Trilinos package today?
- Use integrated analysis to provide real-time feedback:
 - Goals of static analysis tools: Teach, enforce standards & consistency, ...
 - Examples of standards that can checked for automatically:
 - "C++ Coding Standard": Sutter and Alexandrescu
 - "Thyra Coding and Documentation Guidelines"
 - http://www.cs.sandia.gov/~rabartl/ThyraCodingGuideLines.pdf
- Examples of tools that can be integrated into development environment:
 - Separate source analysis tools: AStyle, Google cpplint.py
 - Integrated with GCC compiler:
 - Mozilla Dehydra: https://developer.mozilla.org/en/Dehydra
 - GCC 4.5.x+ plug-in that executes user-defined checks as part of compilation!





Official Trilinos Developers Toolset



Official Trilinos Developers Toolset: Idea and Motivation

- Idea: Define a suite of standard build and other tools along with simple global install script
- Candidate list of software:
 - GCC 4.X.Y (Fortran or no Fortran?)
 - Open MPI ???
 - CMake 2.8.X
 - Git/eg ???
 - CLAPACK ???
 - Boost ???
 - Doxygen ???
 - Graphviz/Dot ???
- Motivation:
 - Reduce variability in development/testing for different developers
 - Turn on strong warnings and warnings as errors!
 - Improve portability of the code
 - Simplify setup of new Trilinos development and test machines
 - Allow more code to be elevated to Primary Stable Code (e.g. boost)





Provide global install script:

\$ Install-trilinos-toolset.py -do-all -install-dir=/home/trilinos/install

- Checks out tarballs from Trilinos3PL CVS repository
- Installs all software in single bin, lib, and include directories
- Uses separate install scripts like install-cmake,py, install-git.py etc.
- Would only support basic Linux (perhaps Unix) and Mac computers (not Windows)

ToDo:

- Decide what software should be included
- Decide on versions of all the software packages
- Refactor existing install-git.py and install-cmake.py to enable faster development of simple install steps
- Get software and write basic install scripts and global install script
- Beta users to work out bugs
- Deploy across all Trilinos developers
- Turn on warnings as errors!
- Enjoy a more stable development environment!





Partitioning of Trilinos Git Repository for Sustained Growth?





Partitioning the "Trilinos" Git Repository?



- Needed for future scalable growth of Trilinos?
- Provides better separation of the Trilinos development community?
- Use git clones to mange currently compatible collections of software?
- Keep integrated with nested Almost Continuous Integration processes

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Page 34 • Need better unit and package-level tests?

Miscellaneous Areas of Needed Improvement and Progress

- Run your own code coverage testing (see TrilinosCMakeQuickstart.txt)
 \$./do-configure -DTrilinos_ENABLE_COVERAGE_TESTING:BOOL=ON
 \$ make dashboard
- Run your own memory checking testing (see TrilinosCMakeQuickstart.txt)
 \$ env CTEST_DO_MEMORY_TESTING=TRUE make dashboard
 - Need a trimmer test suite to allow valgrind to run locally
- Need better namespace safety
 - Don't pollute the global namespace, no 'using namespace ANTHYING'
 - See Trilinos policy on this!
- Need strong warnings and warnings as errors
 - Need a standard version of GCC and MPI first (Official Trilinos Toolset)
- Need to test Doxygen documentation
 - Use some automated HTML testing tools?
- Improving exception safety (basic guarantee, strong guarantee, and no-fail guarantee and memory leaks)
 - Critical for reliable behavior for users
 - Critical for coupling Trilinos code together
- Need more Trilinos Framework staff and scientific programmers to address some of this!



Revised Trilinos Life-Cycle Model?





Definition of Self-Sustaining Software:

- Open source
- High-level document (perhaps just written in Doxygen) describing purpose
- Clean design, clean implementation
- Extremely well tested with unit tests and system verification tests
- Minimal dependencies (all of which are also Self-Sustaining Software)
- (Barely) sufficient documentation
- All maintenance of the software maintains the above properties.

Lean/Agile development methods can create Self-Sustaining Software!





- Allow pure research and applied research with a realistic path to productionization
- Provide smooth low-effort transitions from research to production in phases
- Provide maximum confidence with low cost (for research results and then for real users)
- Allow the use of Lean/Agile practices and processes along the way





- 1) Purely Experimental Code
- 2) Research Stable Code
- 3) Production Growth Stable Code
- 4) Production Maintenance Stable Code

See Trilinos Framework Backlog Item 4837





1) Purely Experimental Code:

- Not developed in a Lean/Agile consistent way
- Could actually be declared to be Secondary Stable code with respect to CI and nightly Trilinos testing but in general would be considered to be Experimental code in Trilinos
- Does **not** provide sufficient unit (or otherwise) testing to prove correctness
- Should **not** be used anything important (not even for research results but in the current CS&E publication environment would be allowed)
- Should not go out in general releases of Trilinos
- Does **not** provide a direct foundation for creating production-quality code

2) Research Stable Code:

- Developed in a Lean/Agile consistent way
- Strong unit and verification testing (i.e. proof of correctness) written while the code/algorithms are being developed
- Could be Primary Stable or Secondary Stable code in Trilinos
- Does **not** generally have good examples, documentation, etc.
- Appropriate to be used by "friendly expert users"
- Appropriate to be part of a general release of Trilinos
- Appropriate to be used in customer codes (with lots of "hand holding")
- Would tend to provide for regulated backward compatibility but not in all cases
- Provides the foundation for creating production-quality code





3) Production Growth Stable Code:

- Includes all the good qualities of "Research Stable Code" plus ...
- Improving validation of user input errors and better error reporting
- Improving formal documentation (Doxygen, technical reports, etc.)
- Improving examples, tutorial material, etc.
- Optional refactoring of the code structure and user interfaces to make more consistent, easier to maintain (should not be needed if software was developed in Agile way)
- Maintain rigorous regulated backward compatibility with few (if any) truly incompatible changes with new releases
- Expanding usage in customer codes
- Appropriate to turn over to a maintenance support team at any time

4) Production Maintenance Stable Code:

- Includes all the good qualities of "Production Growth Stable Code" plus ...
- Primary development only includes bug fixes and performance tweaks
- Maintains rigorous backward compatibility with typically no deprecated features
- Could be maintained by parts of the user community if necessary





THE END

