Software Life-cycle and Integration Issues for CS&E R&D Software and Experiences from Trilinos (Part II, Integration Issues)

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SIAM Parallel Processing 2010, 2/24/2010

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Vision for a Confederation of CS&E Software

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Overview of CS&E Software Engineering Challenge

- Progress in Computational Science and Engineering (CS&E) is occurring due to greater numbers of more complex algorithms and methods
  - **Discretization**: a) meshing, b) advanced discretizations, c) adaptively, …
  - **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) error-estimation, b) stability analysis and bifurcation, c) optimization, d) UQ, …
  - **New architectures**: a) multi-core, b) GPUs, …
  - **Visualization**
  - ...
- Each technology requires specialized PhD-level expertise
- Almost all technologies need to be integrated into single applications
- Set of algorithms/software is too large for any single organization to create
- Too large to be developed under single blanket of Continuous Integration (CI)

Software Engineering and Software Integration are key bottlenecks for CS&E to have the fullest impact!

The Vision: A Confederation of CS&E Codes?

- Develop a confederation of trusted, high-quality, reusable, compatible, software packages/components including capabilities for:
  - **Discretization**: a) meshing, b) advanced discretizations, c) adaptively, …
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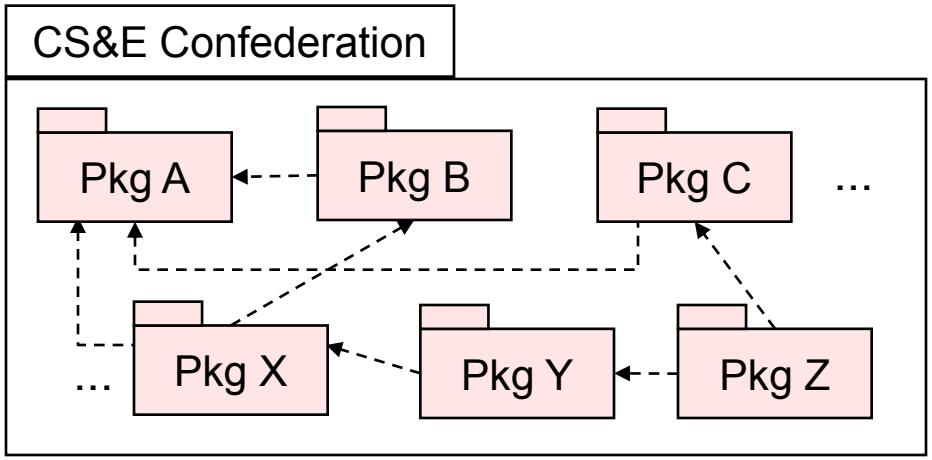

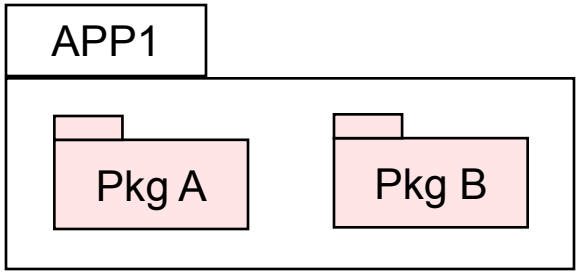

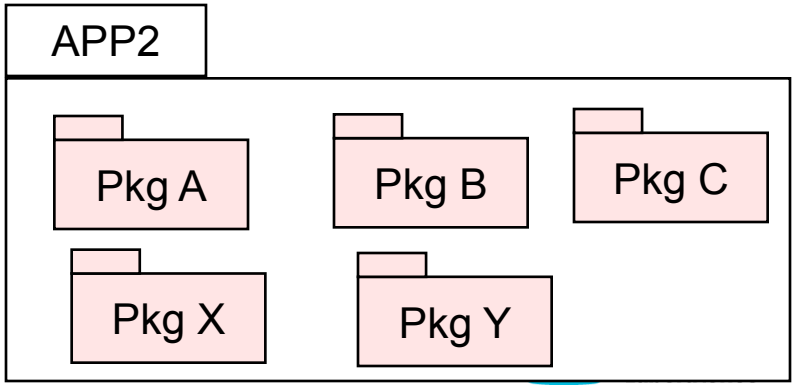

Trilinos itself is a smaller example of this!

Requirements/Challenges for Confederation of CS&E Codes

- Software quality and usability
  - => Design, testing, collaborative development
- Building the software in a consistent way and linking
  - => Common build approach?
- Reusability and interoperability of software components
  - => Incremental Agile design
- Documentation, tutorials, user comprehension
  - => SE education, better documentation and examples
- Critical new functionality development
  - => Closer development and integration models
- Upgrading compatible versions of software
  - => Frequent fixed-time releases
- Safe upgrades of software
  - => Regulated backward compatibility, software quality
- Long term maintenance and support
  - = > Stable organizations, stable projects, stable staff
- Self-sustaining software (clean design, clean implementation, well tested with unit tests and system verification tests) => Anyone can maintain it!

The Trilinos is taking (baby) steps to address all of these issues at some level.

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Software Integration Strategies

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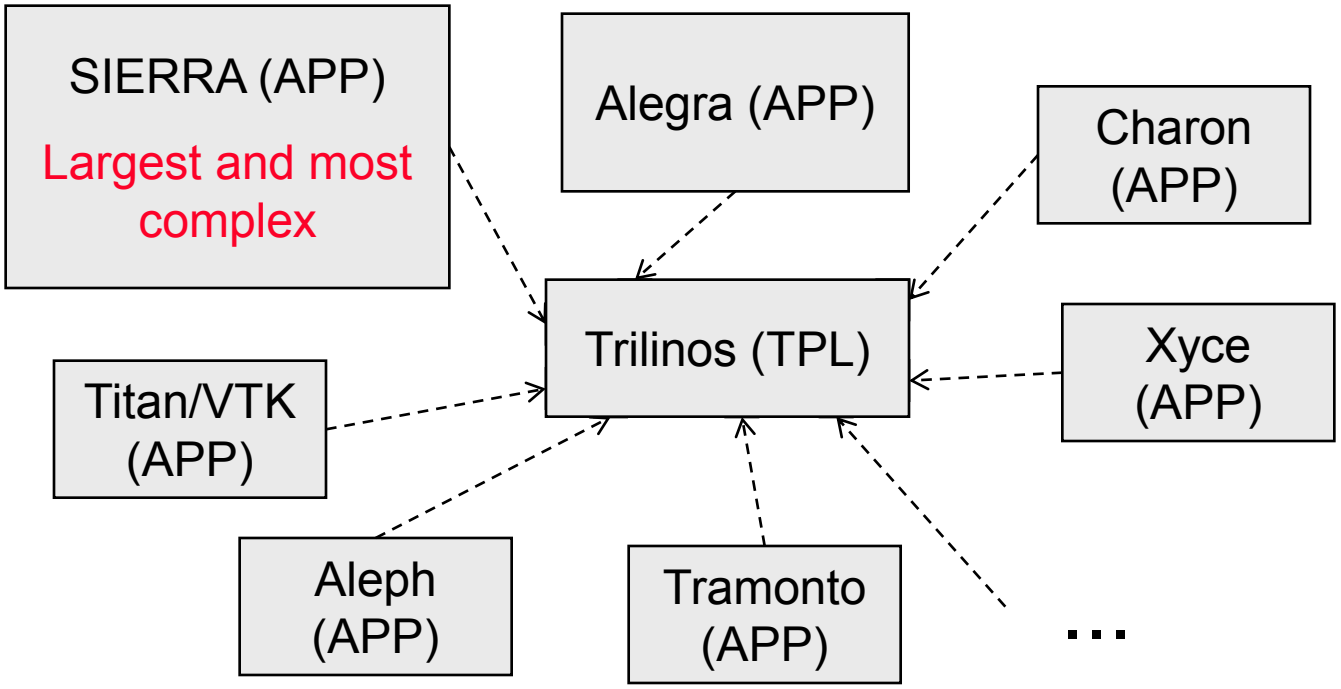
CS&E Environment at Sandia National Labs for Trilinos



TPL: Third Party Lib

- Provides functionality to multiple APPs
- The "Supplier" to the APP

APP: Application

- Delivers end user functionality
- The "Customer" of the TPL

- Sophisticated CS&E applications
  - Discretized PDEs (SIERRA, Alegra, Aleph, Charon)
  - Circuit network models (Xyce)
  - Other types of calculations (Titian/VTK, Tramonto)
- (Massively) parallel MPI (Gordon Bell Winners)
- Almost entirely developed by non-software people
- Wide range of research to production (i.e. from Aleph to SIERRA)

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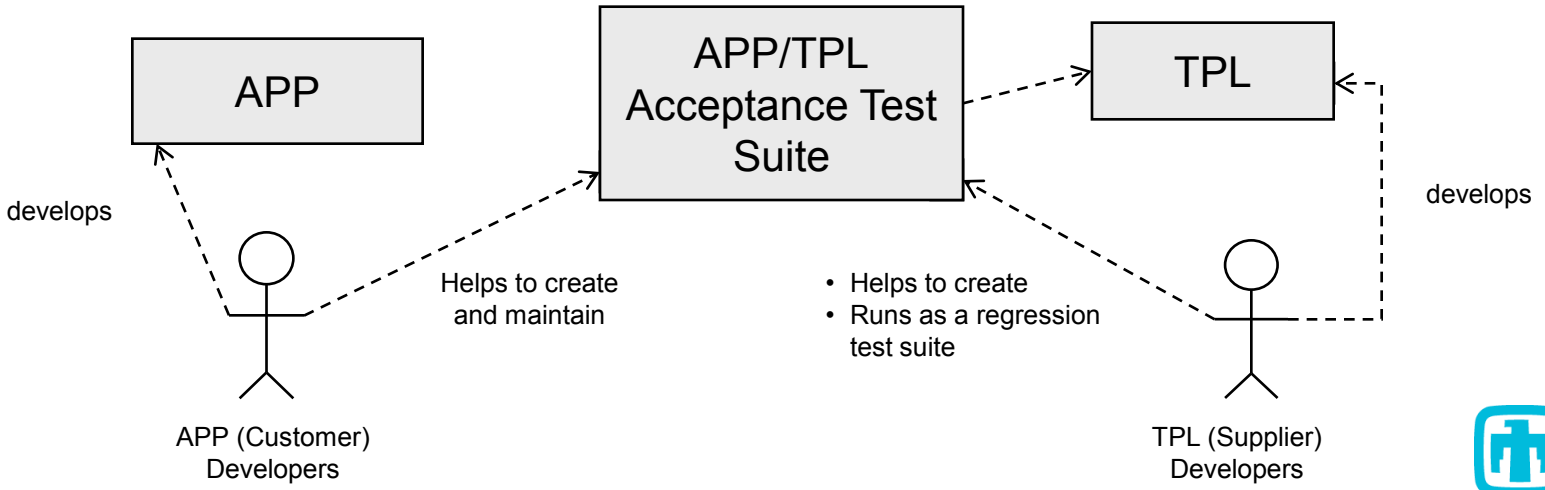
Standard Software Integration Approaches

- Continuous Integration (CI)
  - Code is expected to build and the tests are expected to run
  - Maintained through synchronous or asynchronous CI
  - Requires high levels of cooperation and communication
  - Requires code to (re)build fast and tests to run fast

- Customer/Supplier Relationships
  - Combined code too large to build under single CI system
  - Organizations can not cooperate close enough
  - Protect APP for future TPL updates through development of Acceptance Test Suite
  - May not work as well for may CS&E codes
  - Not as well suited for closer collaborations



Special Challenges with CS&E Software

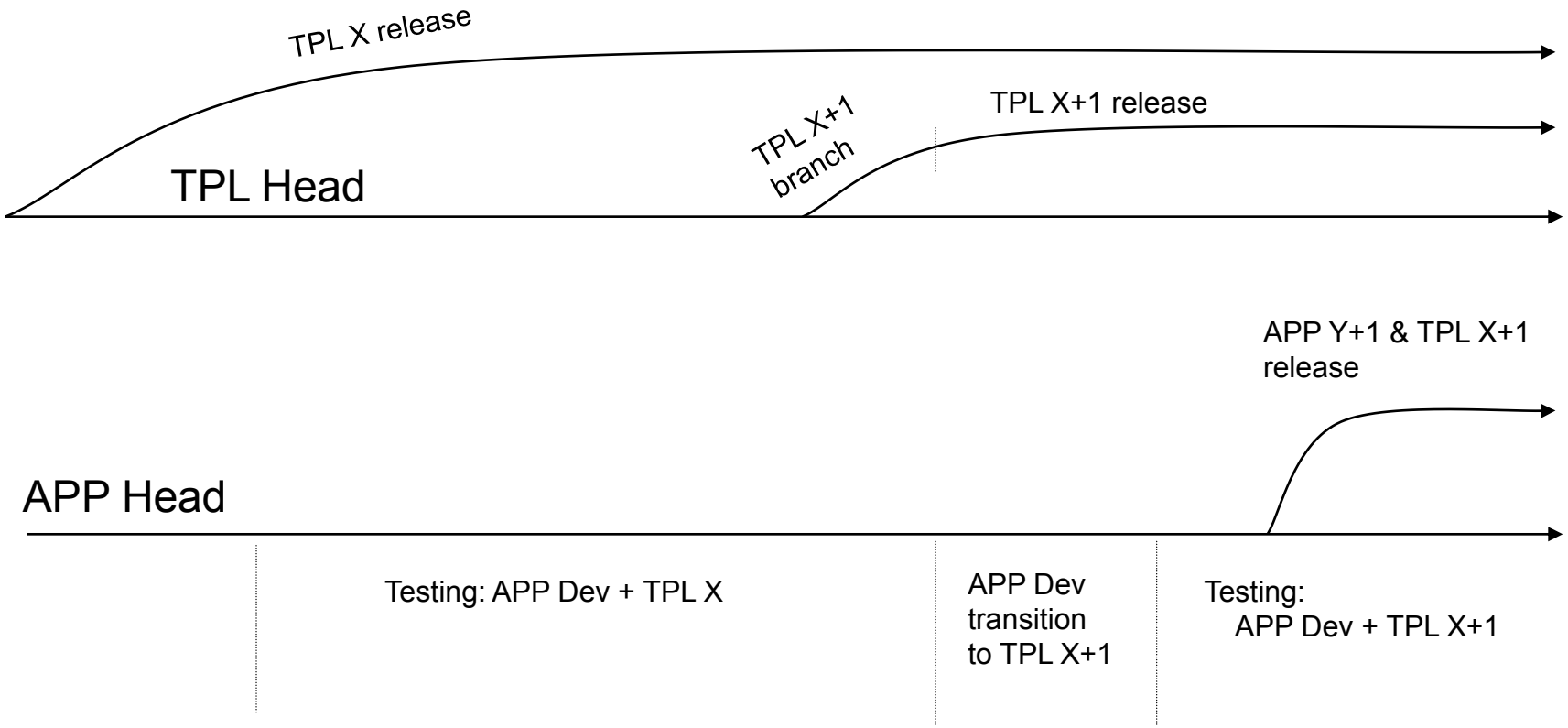
- CS&E heavily relies on fast floating-point computations
  - Output from program varies between platforms and even with different compiler options!
  - How to you keep tests working on different platforms?
- CS&E involves complex nonlinear models
  - Examples: ill conditioning, multiple solutions, bifurcations, non-convexities ...

These issues conspire together to make testing and maintaining CS&E software on multiple platforms very difficult!

Consequences:

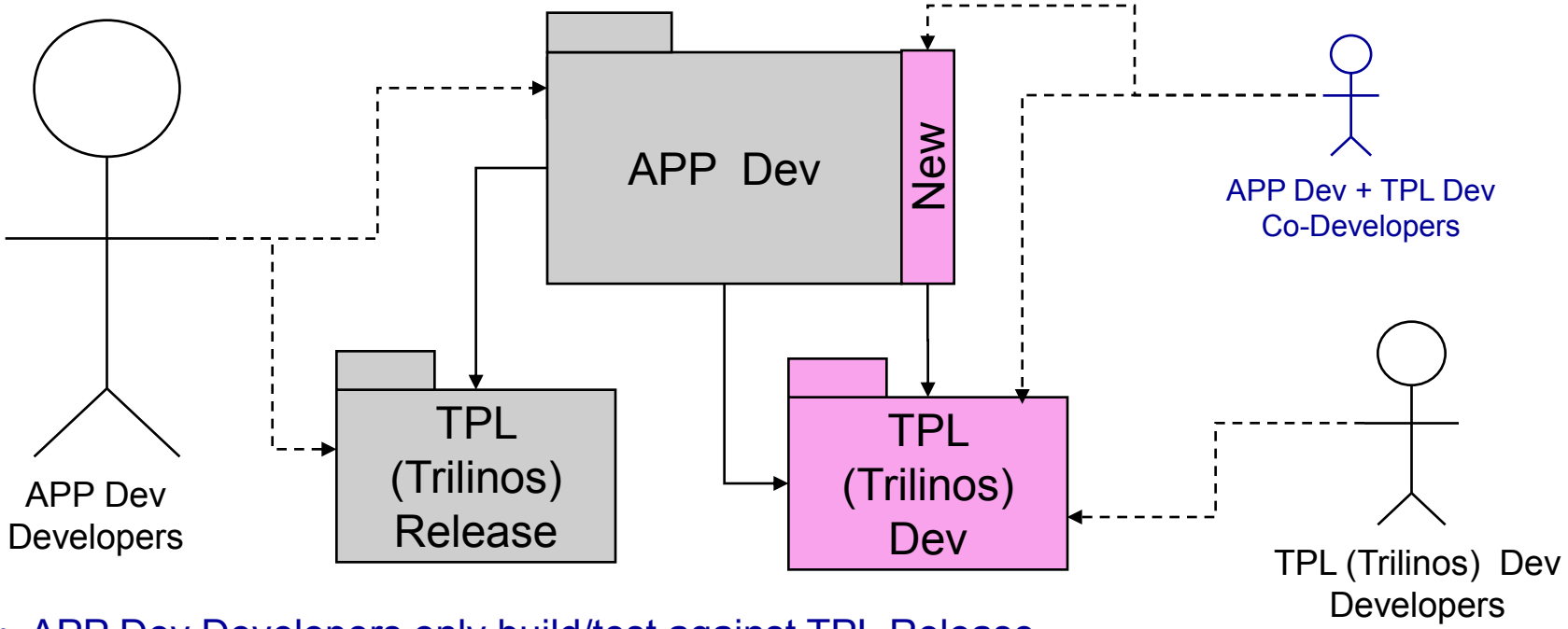
- A new test status: The diffing test!
  - Code runs to completion but some error tolerance was exceeded
  - Many CS&E practitioners convince themselves that a “diff” is not as bad as a “fail”!
- Changes to a numerical algorithm that improve performance in every measure can cause numerous tests to ‘diff’ or even ‘fail’!
- Upgrades of a TPL can break an APP even if no real defects have been introduced!

APP + TPL Release with Punctuated TPL Upgrades



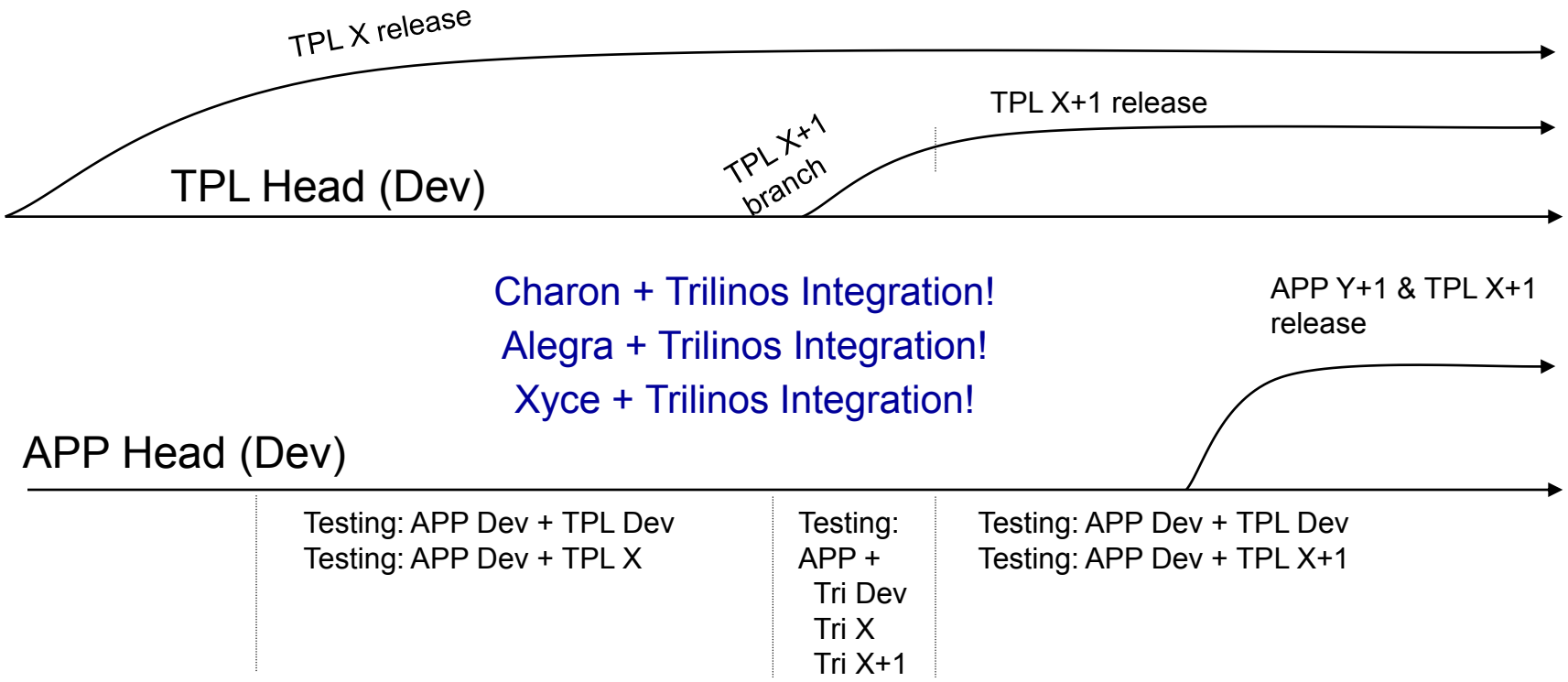
- Transition from TPL X to TPL X+1 can be difficult and open ended
- Large batches of changes between integrations
- Greater risk of experiencing real regressions
- Upgrades may need to be completely abandoned in extreme cases
- However, this is satisfactory for many APP+TPL efforts!

APP + TPL Release and Dev Daily Integration



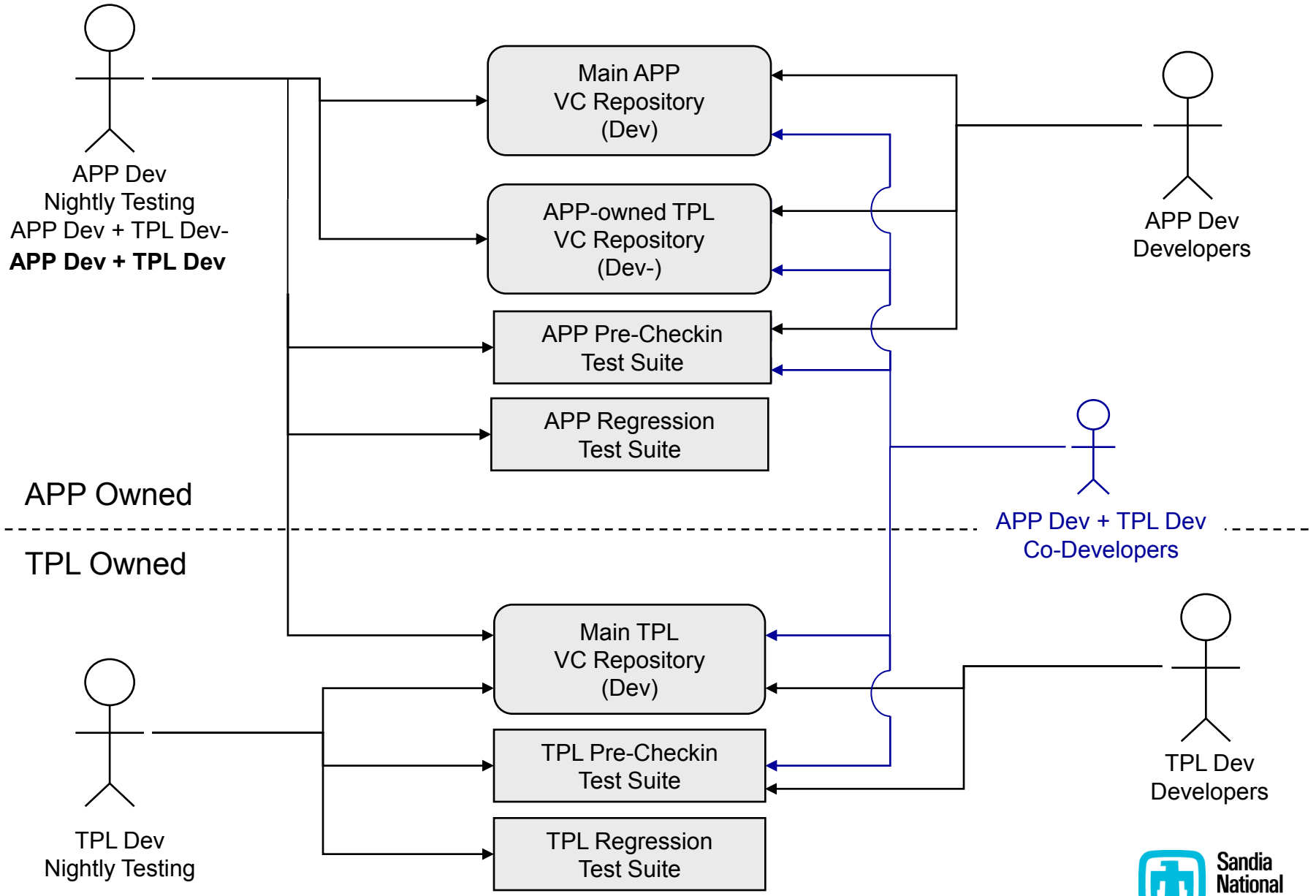
- APP Dev Developers only build/test against TPL Release
- TPL (Trilinos) Dev Developers work independent from APP
- Keep APP Dev and TPL Dev up to date! => Supported by TPL backward Compatibility!
- Use of staggered releases of TPL and APP
- APP + TPL Dev Co-Developers drive new capabilities
- Difficult for APP to depend too much on TPL
- Does not support tighter levels of integration and collaboration
- APP developers can break “New” a lot when refactoring
- However, this is satisfactory for many APP+TPL efforts!

APP + TPL Release and Dev Daily Integration



- All changes are tested in small batches
- Low probability of experiencing a regression
- Extra computing resources to test against 2 (3) versions of TPL
- Some difficulty flagging regressions of APP + TPL Dev
- APP developers often break APP + TPL Dev when refactoring
- Difficult for APP to rely on TPL too much
- Hard to verify TPL for APP before APP release
- However, this is satisfactory for many APP+TPL efforts!

APP + TPL Almost Continuous Integration: Overview



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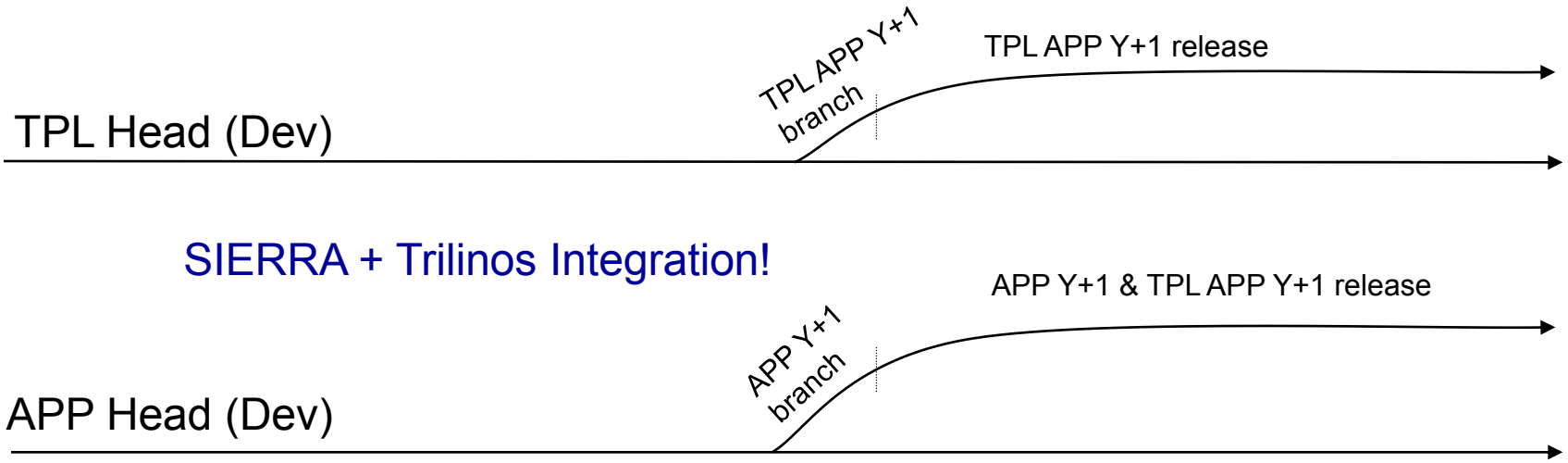
APP + TPL Almost Continuous Integration: Releases



Nightly Testing: APP Dev + TPL Dev (pre-checkin tests only, TPL Dev- checkin)
Nightly Testing: APP Dev + TPL Dev- (complete test suites)
Supported with asynchronous continuous integration testing of APP Dev + TPL Dev

- All changes are tested in small batches
- Low probability of experiencing a regression between major releases
- Less computing resources for detailed nightly testing (only one TPL version)
- All tested regressions are flagged in less than 24 hours
- Allows code to flow freely between the APP and TPL
- Supports rapid development of new capabilities from top to bottom
- All code checked out by APP Dev developers has passed pre-checkin build/test
- More complex processes (i.e. requires some tools?)
- APP Dev developers spend more time spent recompiling TPL code
- Recommended for projects requiring high levels of integration & collaboration!

APP + TPL Integration: Different Collaboration Models

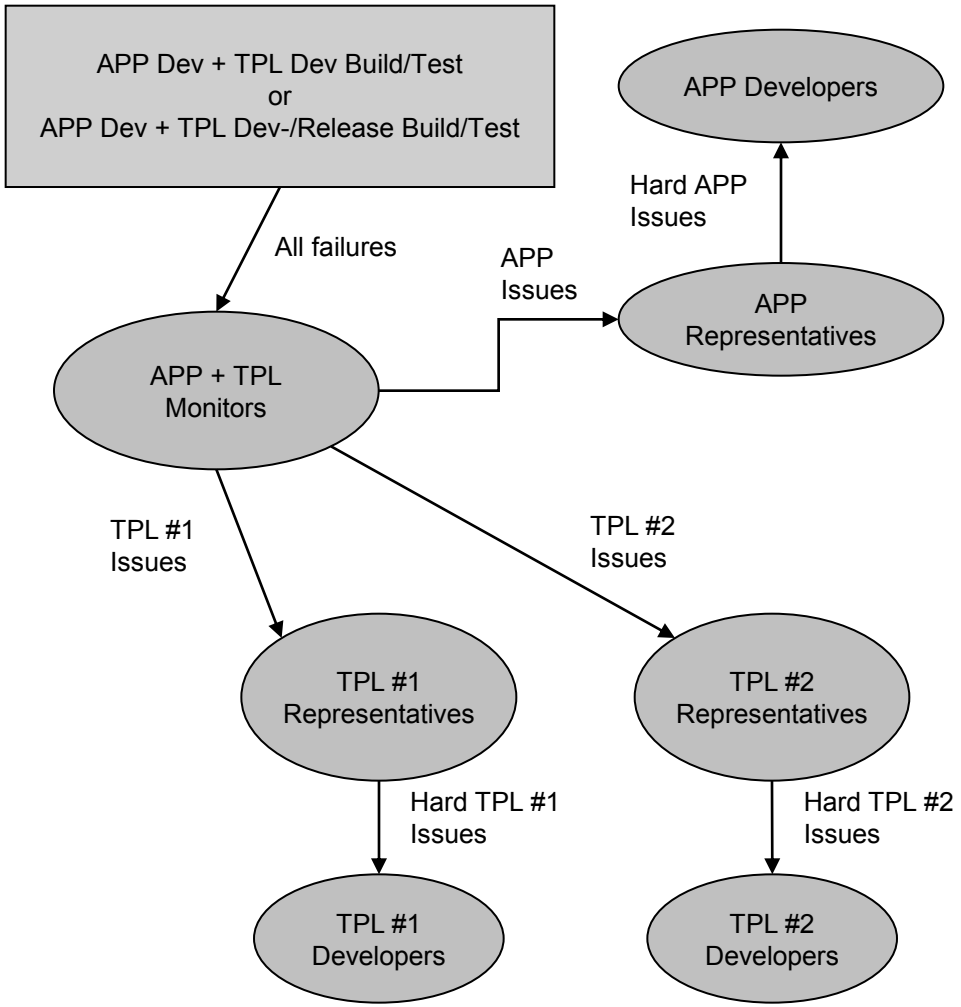
- Absorb sources for TPL and never upgrade
  - Just a code seeding strategy and not an integration strategy
- APP + TPL Release with Punctuated TPL Upgrades
  - Little to no testing of APP + TPL Dev in between versions
- APP + TPL Release and Dev Daily Integration
  - APP developers work against TPL Release
  - APP + TPL team(s) build against TPL Dev
  - Nightly and CI testing done for both APP + TPL Release and Dev
  - Must handled staggered releases of TPL and APP
- APP + TPL Almost Continuous Integration
  - APP developers work directly against TPL Dev checked out every day
  - Releases best handled as combined releases of APP and TPL

Selecting an Integration Model for CS&E Software

- Each of these different integration models will be appropriate for a particular APP+TPL situation.

- The particular integration model can be switched during the life-cycles of the APP and TPL depending on several factors:
  - Level of dependence on TPL?
  - Level of duplication of functionality in TPL with other external packages?
  - Level of sophistication of TPL?
  - Ease or difficulty of independent verification of TPL?
  - Level of active development of TPL?
  - Need for new functionality and upgrades of TPL?
  - Interdependence of TPL on other external software packages?
  - Level of quality needed for TPL?
  - Level of Software Quality Engineering used to produce TPL?
  - Release schedule for TPL?
  - Level of relationship and pull with the developers of TPL?
  - Stability of the organization that develops and supports TPL?
  - Usage of TPL by other related sister codes?
  - ...

Maintenance of APP + TPL Integration



- APP + TPL Monitor:
  - Member of the APP development team
  - Has good familiarity with the TPLs
  - Performs first-round triage (APP or TPL?)
  - Forwards issues to APP or TPL Reps
  - Ultimate responsibility to make sure issues are resolved
- APP Representative:
  - Member of the APP development team
  - Second-round triage of APP issues
  - Forwards hard APP issues to APP developers
- TPL Representative:
  - Member of the TPL development team
  - Has some familiarity with the APPs
  - Second-round triage for TPL issues
  - Forwards hard TPL issues to TPL developers
- General principles:
  - Roles of authority and accountability (Ordained by management)
  - At least two people serve in each role
  - Rotate people in roles

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Summary

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Summary of CS&E Software Integration Models

- Nightly building and testing of the development versions of the application and TPLs:
  - results in better production capabilities and better research,
  - brings TPL developers and APP developers closer together allowing for a better exchange of ideas and concerns,
  - refocuses TPL developers on customer efforts,
  - helps drive continued research-quality TPL development, and
  - reduces barriers for new TPL algorithms to have impact on production applications.
- Integration Models:
  - APP + TPL Release with Punctuated TPL Upgrades
    - Little to no testing of APP + TPL Dev in between TPL releases
  - APP + TPL Release and Dev Daily Integration
    - Daily Integration testing done for both APP + TPL Release and Dev
    - Staggered releases of TPL and APP
  - APP + TPL Almost Continuous Integration
    - APP Dev + TPL Dev developers update both APP-owned and main TPL repositories
    - Nightly testing of APP Dev + TPL Dev automatically updates APP-owned TPL Dev- VC Repository
    - Releases best handled as combined releases of APP and TPL
    - TPL Dev- checkins can be dialed back approaching TPL Release and Dev Integration!

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Possible topics for Round Table Discussion at 6:00 PM

THE END

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