Integration Strategies for Computational Science & Engineering Software

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Software Integration in the CS&E Environment

- Need to integrate a large amount of CS&E software:
  - Meshing
  - Discretizations
  - Solvers
  - Adaptivity
  - Analysis capabilities
  - Visualization
  - ...
- Each CS&E discipline is highly specialized and requires PhD-level expertise
- The set of algorithms and software is too large for any single organization to produce
- Set of software is too large to be developed under a single blanket of Full Continuous Integration (CI)

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

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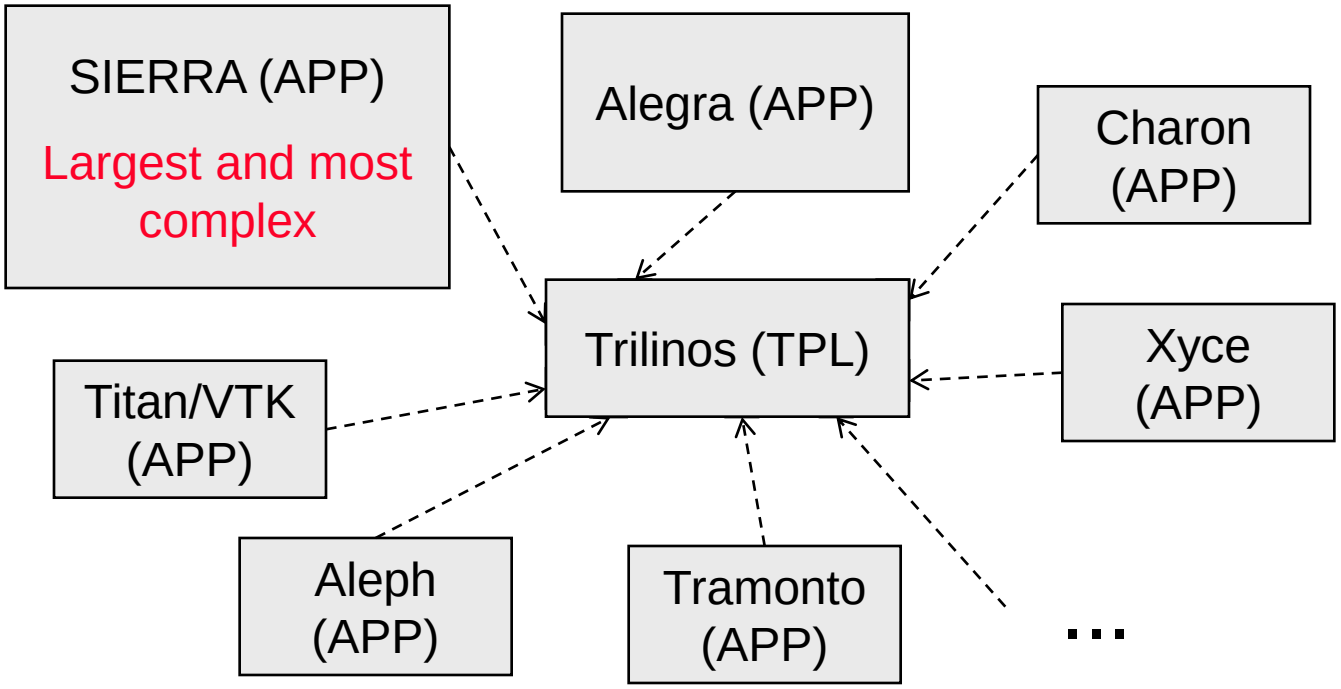
CS&E Environment at Sandia National Labs for Trilinos



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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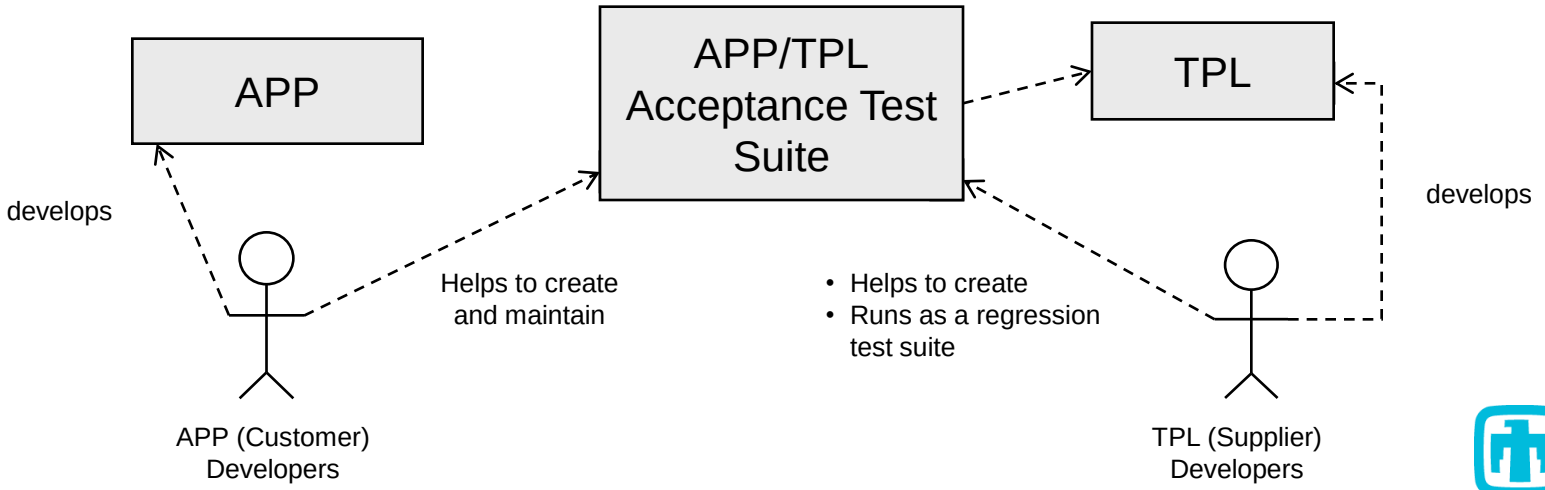
Standard Software Integration Approaches

- 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



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Challenges to Software Integration in CS&E Environments

- CS&E is a mix of research and production work
  - How can you mix research and production software?
- CS&E practitioners have a wide mix of backgrounds in physics, math, computer science, engineering, etc.
  - How to these people communicate together and integrate their technologies?
- CS&E involved very complex, very specialized algorithms
  - Requires PhD in area to develop best algorithms/software
  - How to integrate very different complex algorithms software?
- Great variability in knowledge and interests in basic software development knowledge and skills
  - How can you produce high quality trusted software with unskilled programmers?
- Close collaboration between different disciplines needed to solve the hard problems
  - How can different practitioners work together through their 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 ...

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!

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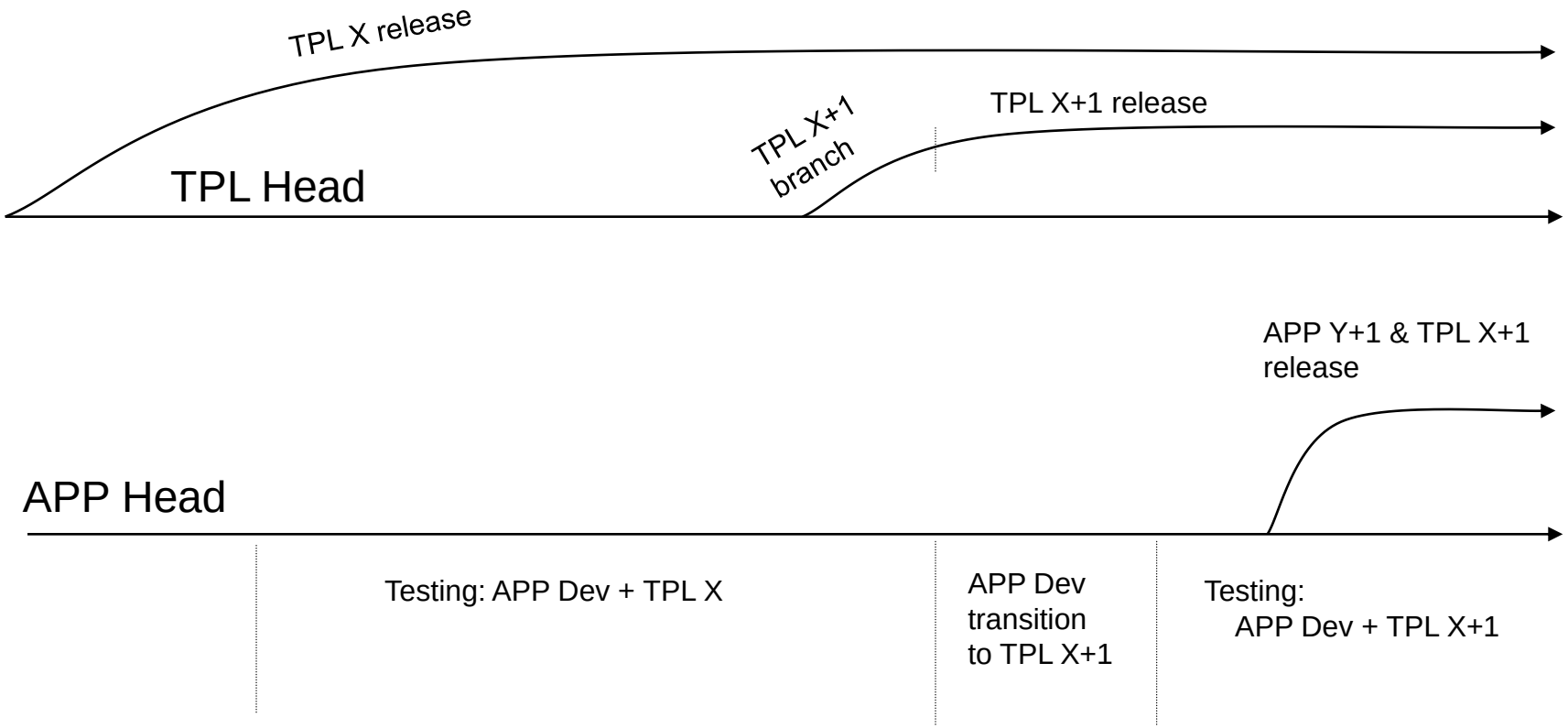
APP + TPL Release with Punctuated TPL Upgrades



- 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!

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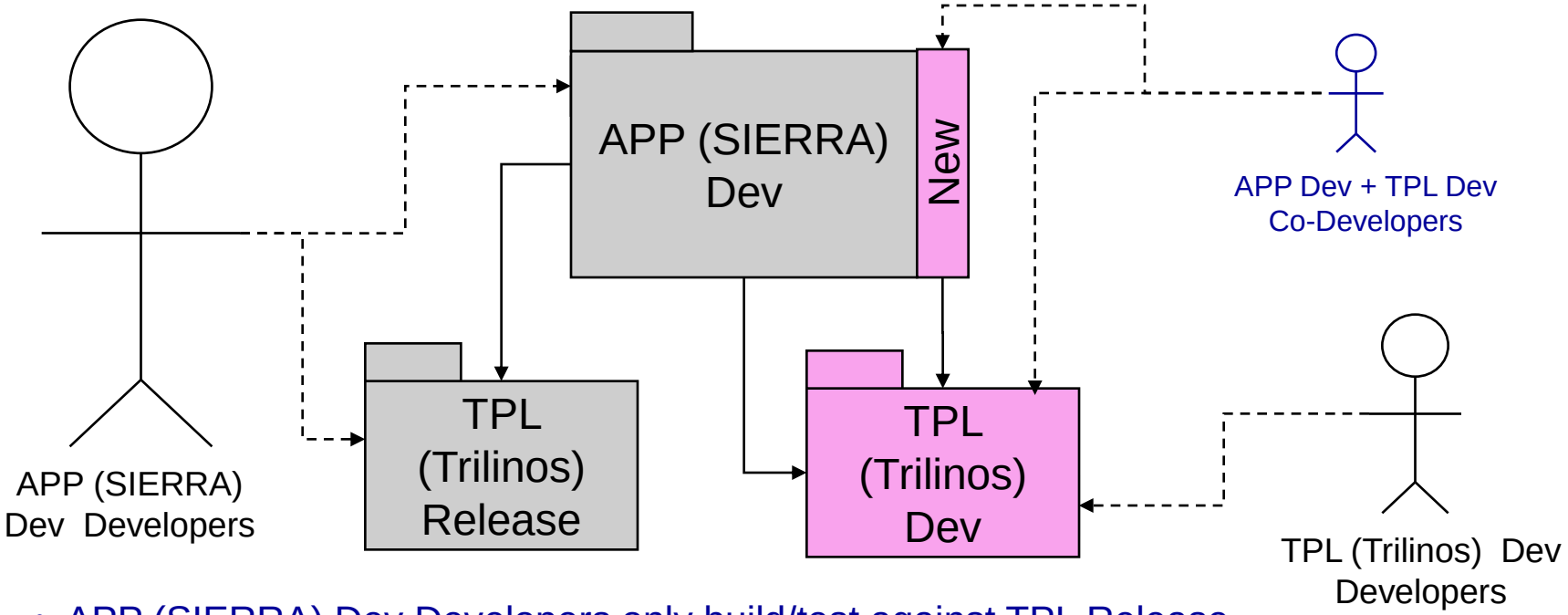
APP + TPL Release and Dev Daily Integration



- APP (SIERRA) 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 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!

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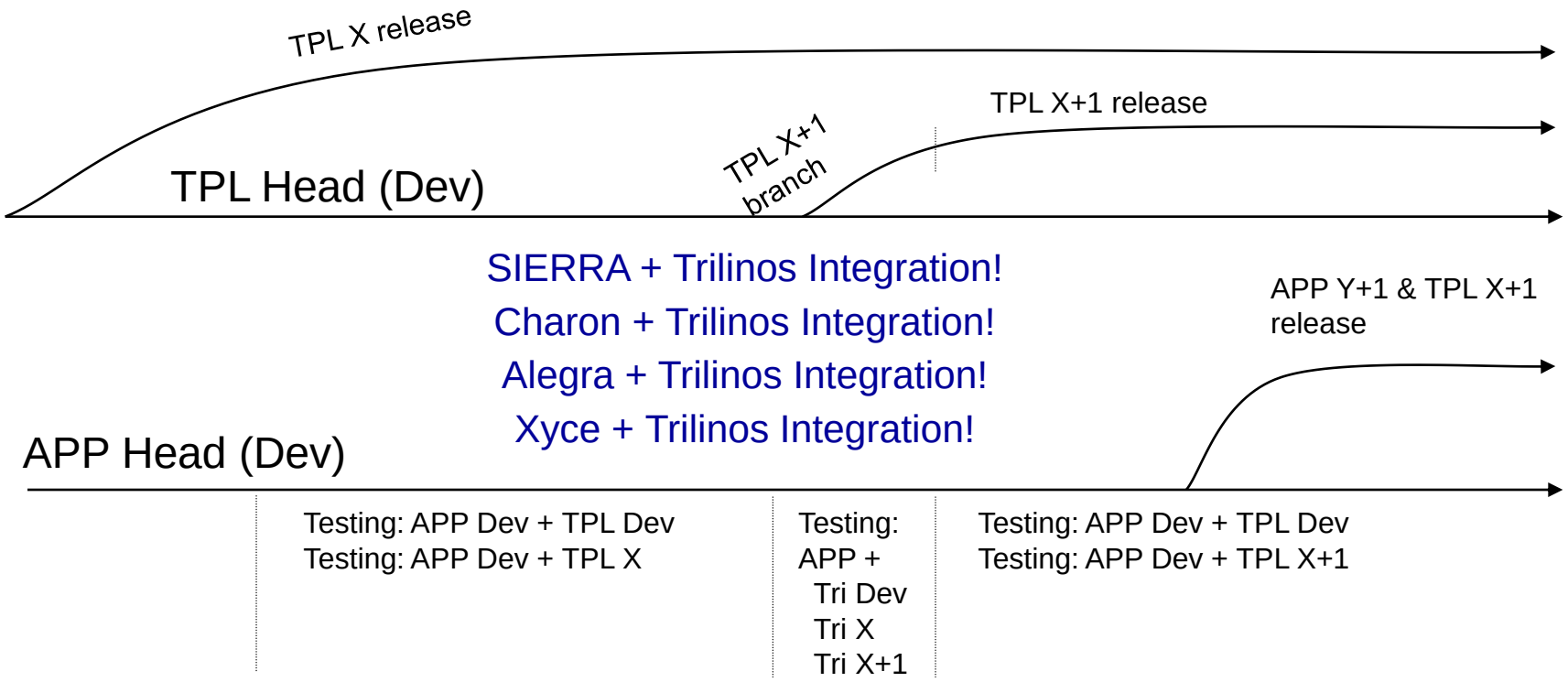
APP + TPL Release and Dev Daily Integration



- 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: Principles

- Regular TPL developers only build and run TPL pre-checkin test suite.
- Regular APP developers should only check out code that has already built and passed their pre-checkin APP test suite.
- Code that builds and passes the pre-checkin test suite is safe to check in.
- Co-development of the APP + TPL needs to be productive and not discourage frequent checkins (at least to direct collaborators).
- Regular APP developers should be able to easily build and test “New” APP + TPL Dev code to avoid breaking it before checkin.

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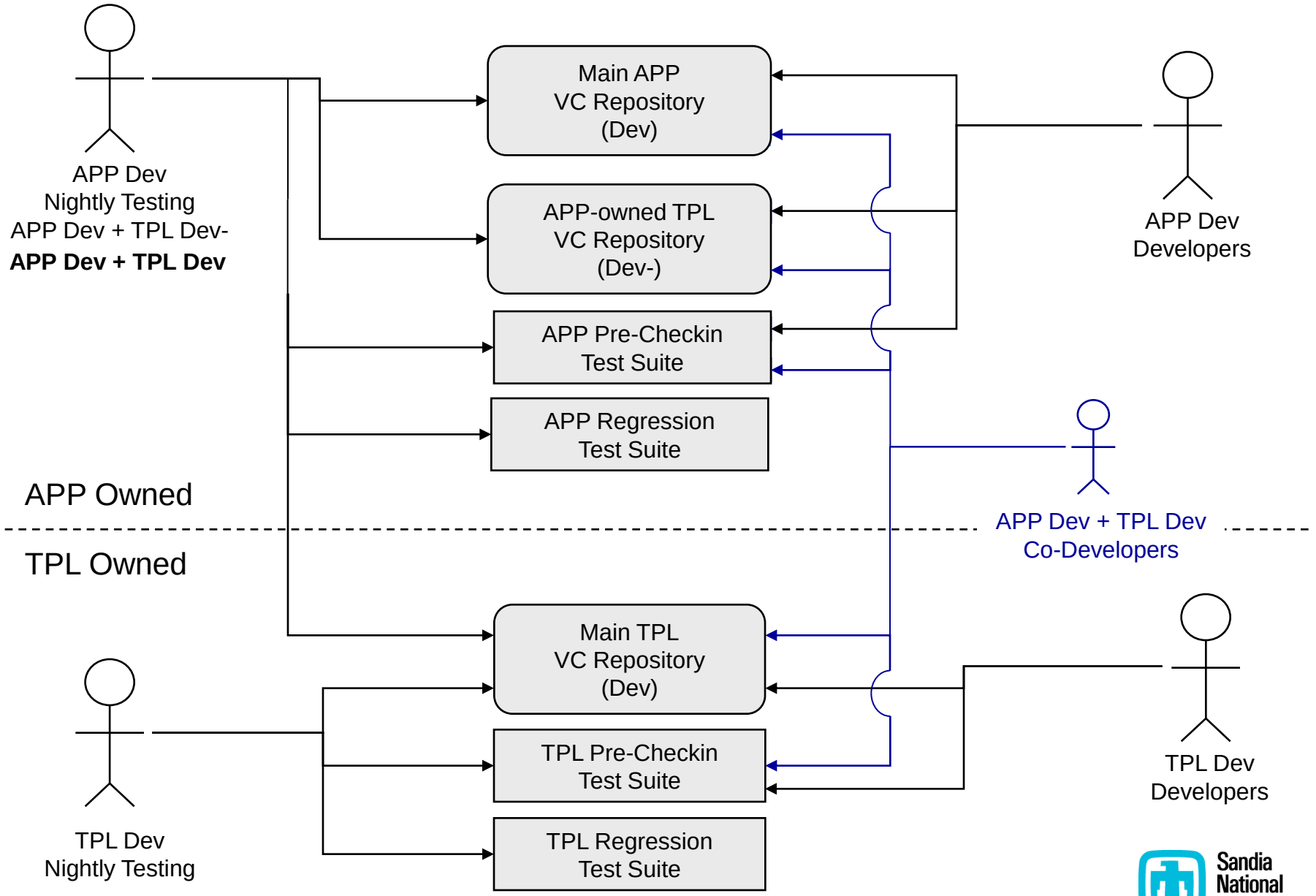
APP + TPL Almost Continuous Integration: Overview



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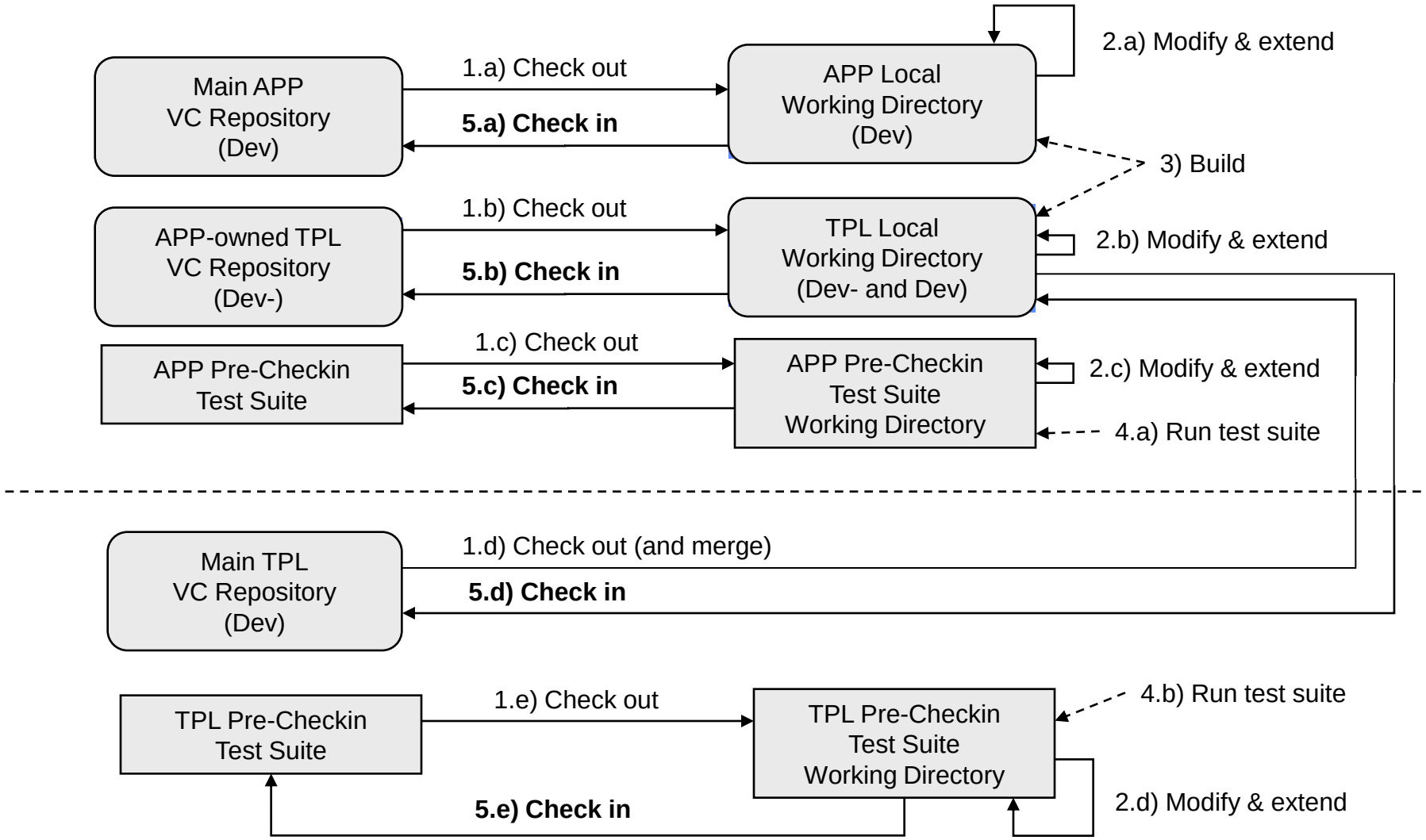
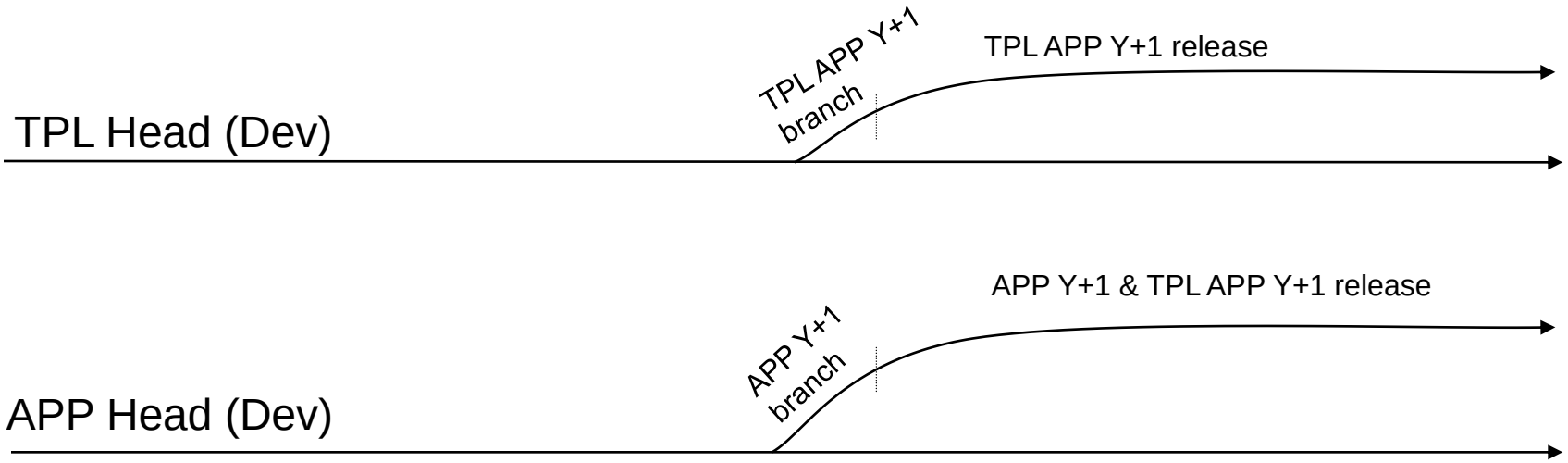
APP + TPL Almost Continuous Integration: Co-Development



- Pre-checkin test suites for APP and TPL are both run before checkin
- Simultaneous checks into APP-owned TPL Dev- and Main TPL Dev VC Repositories!
  - Changes in APP-owned TPL VC Dev- Repos get back into Main TPL VC Dev Repos!

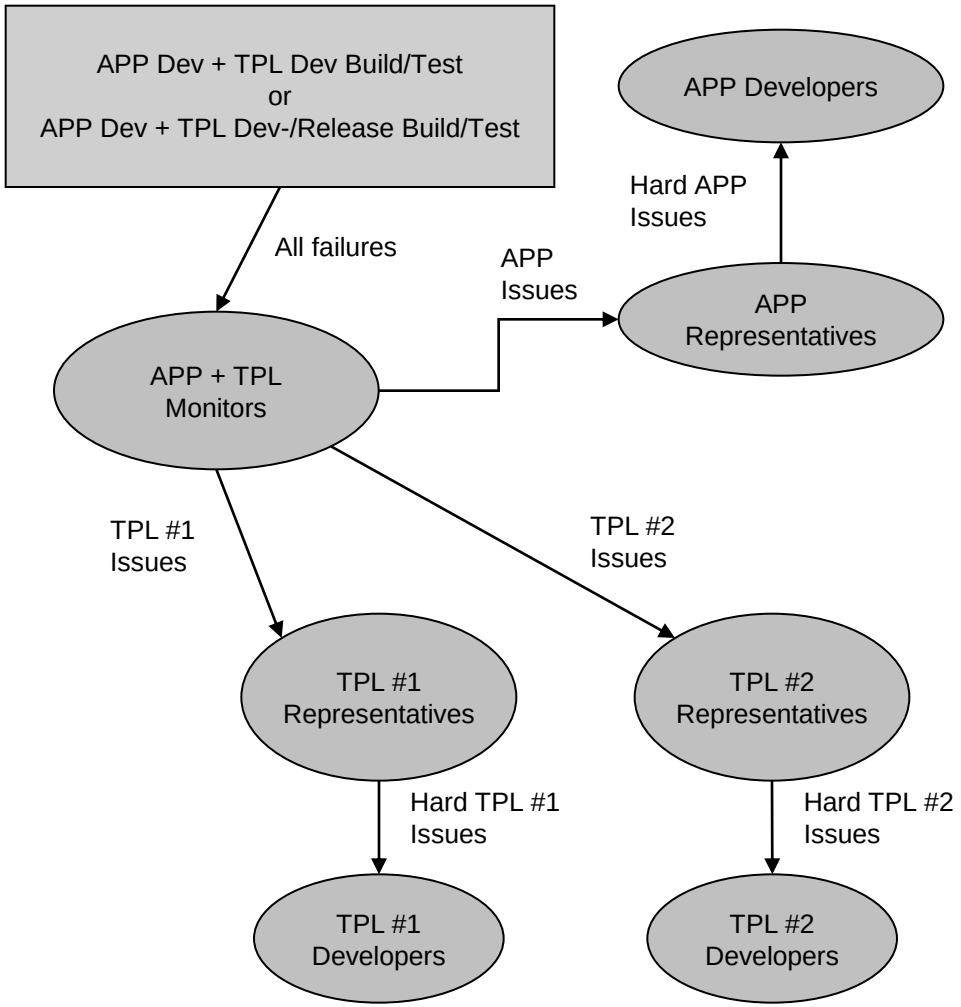
APP + TPL Almost Continuous Integration: Releases



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!

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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Experience with Integration Approaches with Trilinos at SNL

Charon + Trilinos Integration:

- First implemented APP + TPL Release and Dev Daily Integration in 2007
- Maintained daily integration with little effort
- Supporting more ambitious collaborations and integration efforts
- However, has never gone through a full release process under this model

- Alegra + Trilinos Integration:
  - Started APP + TPL Release and Dev Daily Integration in 2008
  - Maintained daily integration with little effort on multiple platforms
  - Upgrade to Trilinos 9.0 was easy and risk free, less overall effort
- SIERRA + Trilinos Integration:
  - Started APP + TPL Release and Dev Daily Integration in mid 2008
  - Before daily integration:
    - SIERRA 4.9 released against Trilinos 7.0 (a 1.5 year old release)
    - Upgrade of SIERRA VOTD to Trilinos 8.0 was a “disaster”
  - After daily integration:
    - SIERRA 4.10 released against Trilinos 9.0 (2 months old) with no issues
    - SIERRA 4.11 released against snapshot branch of Trilinos (2 weeks old)
  - Currently having lots of problems with broken code in “New” APP code
  - APP + TPL Almost Continuous Integration Process currently being developed!

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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:
  - How critical is the TPL functionality currently to the APP?
  - Are there alternatives to a particular TPL that can duplicate functionality?
  - How actively is the TPL being developed?
  - Is it critical for the APP to continue to accept new releases of the TPL?
  - How active is the collaboration between APP and TPL developers?
  - Is the TPL a fundamental part of the infrastructure of the APP?
  - ...

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Conclusions

- Need to integrate a large amount of CS&E software:
  - Meshing
  - Discretizations
  - Solvers
  - Adaptivity
  - Analysis capabilities
  - Visualization
  - ...
- Software Engineering and Software Integration are key bottlenecks for CS&E to have the fullest impact!
- The CS&E R&D community needs to adopt better Lean/Agile software engineering methods:
  - Need a strategy to inject basic software engineering knowledge into CS&E
  - These methods must be adapted to the special properties of CS&E

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The End

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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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