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Better Scientific Software tutorial @ SC22

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- Individual modules may be cited as *Speaker, Module Title*, in Better Scientific Software tutorial, ...

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Why Develop Software Collaboratively?

- Most real-world projects involve teams rather than individuals
- Collaboration has advantages
 - Produces working code quicker
 - Better design from considering more points of view and experience
 - Can be more enjoyable, even a social experience
- Collaboration has challenges
 - Logistics (time zones etc.)
 - Communication
 - Ensuring everyone is working from the same version and can contribute equally
 - Understanding other's code and what they intended





Why do we need tools?

Kanban feature branch

- To keep organized when working on a team
- Stay on the same page, same knowledge of the project, work, goals etc.
- Keep track of, address and prioritize bug fixes, feature requests, etc.



Version Control - Git

- Version control (or revision control) is a means of tracking changes made to source code
- Various hosting services are available GitHub, GitLab, Bitbucket, etc.
- Main features of Git used for collaboration*
 - Branches allows separate development for features or fixes on the same repo
 - Pull Requests (PRs) Enables code review and testing before merge
 - Clones allows each developer their own working copy
 - Forks allows those outside the team to collaborate (open source software)

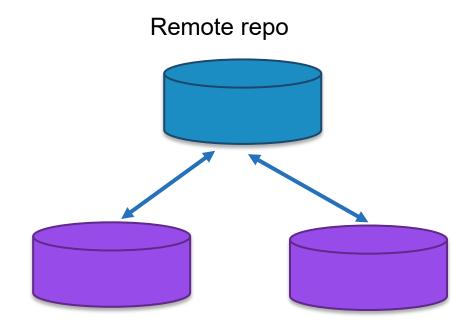
* This tutorial will cover the first two since knowledge of them is needed for the development workflow using Git, referred to as "Git Workflow"





Version Control - Git

Allows collaboration while ensuring everyone works from the same version









Use of Branches

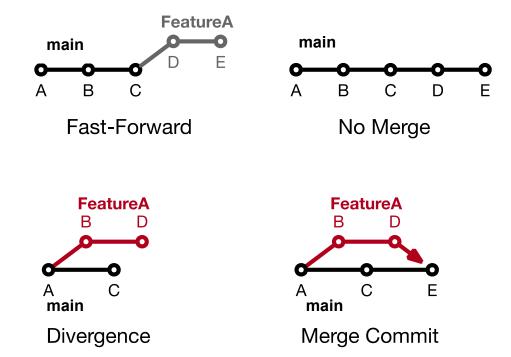
- Enables independent development for features or fixes on the same repo
- Enables concurrent development by multiple developers
- Provides different types of Workflows
- Protects main branch
- Develop on a branch, test on the branch, and merge into main
- Integration occurs at merge commits





Feature Branches

Organize a new feature as a sequence of related commits in a branch







How Do We Control Project Branch Complexity?

- Workflow policy is needed
 - Project supported branches and workflows should not be unnecessarily complex
 - Individuals and sub-teams can leverage more complex models when advantageous
 - Descriptive names or names linked to issue tracking system
 - Where do branches start and end?

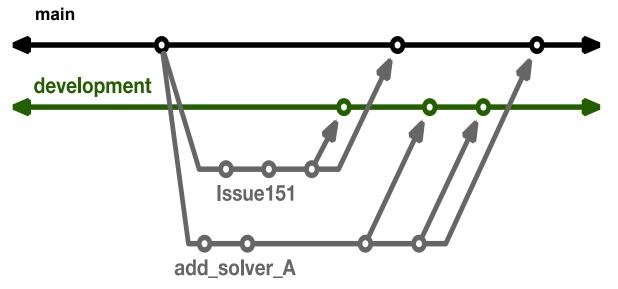






Infinite Lifetime Branches

- Base off main branch
- Exist in all copies of a repository
- Each provides a distinct environment
 - Development vs. pre-production







Branching Strategies

- What's stable, under what conditions?
- What's tested?
- Branch Lifetimes
 - Indefinite main, development, stable
 - Short term feature, fixes
 - Longer Period based on release schedules
- Establish Workflow Policies





Pull Requests

Why use Pull Requests?

- Allows code review and testing before merge
 - Alerts team and others about changes in branch before merge
 - Discussions ensue with possible follow up commits
 - Can request reviewer (may want particular expertise, may want to give someone knowlege)
- Set policies for merge
 - Enforce rules such as coding standards
 - Minimum number of reviewers
 - Protected branches who can merge to certain branches etc.





What makes a good Pull Request?

- Covers "one thing"
 - One body of work
 - Independently manageable
- Avoid large PR's keep them small
- Break them up if they get too large
- Merge frequently (goes with keep them small)
- Good description helps reviewers and users





What is a Git Workflow?

- A Git workflow consists of the structure of the branches and policies
 - Designated lifetime branches
 - main, production, pre-production, development
 - Feature Branches
 - New features, bug fixes etc.
 - Schedules for releases (if applicable)
 - Testing
 - Branch Protections





Why use a Git Workflow?

- Provides collaboration in a consistent and productive manner
- Team members are on the same page for development
- Policies make it clear
 - How to use the branching structure
 - What branches are protected
 - What is tested and when
 - What branches are stable
- Helps team members understand the current state of the code





Commonly Known Git Workflows

- Git Flow
- GitHub Flow
- GitLab Flow

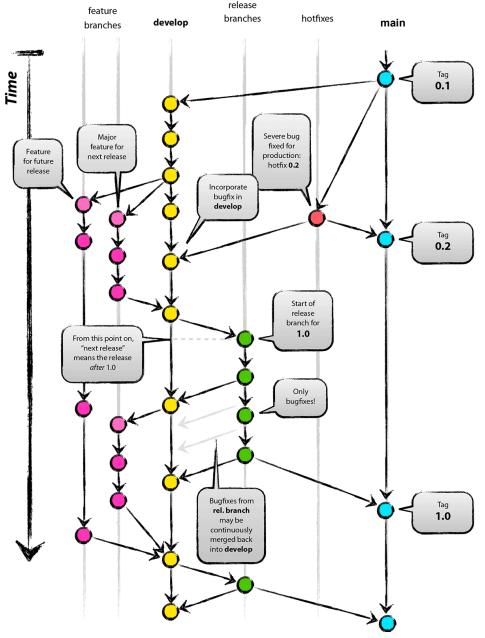
Extra Slides at the end show real Git Workflows of some CSE projects

<u>Design Patterns for Git Workflows</u> by Roscoe A. Bartlett provides an extensive discussion of the concepts behind git workflows





Git Flow



- Full-featured workflow
- Increased complexity
- Designed for SW with official releases
- Feature branches based off of develop
- Git extensions to enforce policy
- How are develop and main synchronized?
- Where do merge conflicts occur and how are they resolved?

Author: Vincent Driessen

Original Blog: https://nvie.com/posts/a-successful-git-branching-model/

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GitHub Flow

http://scottchacon.com/2011/08/31/github-flow.html

- Published as viable alternative to Git Flow
- No structured release schedule
- Continuous deployment & continuous integration allows for simpler workflow

Key Ideas

- 1. All commits in the main branch are deployable
- Base feature branches off of main
- 3. Push local repository to remote constantly
- 4. Open Pull Requests early to start dialogue
- 5. Merge into main after Pull Request review





GitLab Flow

https://docs.gitlab.com/ee/workflow/gitlab_flow.html

- Published as viable alternative to Git Flow & GitHub Flow
- Semi-structured release schedule
- Workflow that simplifies difficulties and common failures in synchronizing infinite lifetime branches

Key Ideas

- main branch is staging area
- Mature code in main flows downstream into pre-production & production infinite lifetime branches
- Allow for release branches with downstream flow
 - Fixes made upstream & merged into main.
 - Fixes cherry picked into release branch





Guidelines for establishing a Git Workflow

- Communicating it to your collaborators
 - Include workflow in Contributing Guide
 - Establish conventions for branch naming (issues, major/minor versions)
- Enforce workflow
 - Branch protections
 - Limiting who can push/merge
 - Testing & review requirements
- Adopt what is good for your team
 - Consider team culture and project challenges
 - Assess what is and isn't feasible/acceptable
 - Start with simplest and add complexity where and when necessary





Why Agile?

- Fits the research experience better than heavier-weight approaches
 - Aligns more naturally with how scientific progress is made
- Well-suited for scientific software efforts (when tailored correctly)
 - Works well for small teams
 - Provides meaningful, beneficial structure that promotes
 - Productivity
 - Productization
 - Sustainability
 - Flexibility in requirements
 - Communication





What is Agile?

- Agile is not a software development lifecycle model
- Agile is informally defined as
 - I don't write documentation
 - I don't do formal requirements, design, or really test...
 - Agile is not an excuse to do sloppy work
- Some people consider agile to be synonymous with Scrum
 - From Atlassian: Scrum is a framework that helps teams work together
 - Scrum is Agile, Agile is not (only) Scrum
 - A square is a rectangle, not all rectangles are squares
 - Agile is not Kanban either





What is Agile?

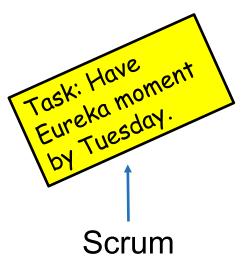
http://agilemanifesto.org/



Getting Started with Agile

- Agile principles are not hard and fast rules
- Try adopting a few Agile practices
 - Following a rigid, ill-fit framework usually leads to failure

- Kanban is a good starting framework
 - Follow basic principles, add practices when advantageous
 - Better than removing elements from Scrum







Basic Kanban

Backlog	Ready	In Progress	Done
 Any task idea Trim occasionally Source for other columns 	 Task + description of how to do it. Could be pulled when slot opens. Typically comes 	 Task you are working on right now. The only Kanban rule: Can have only so many "In Progress" tasks. Limit is based on experience, calibration. 	 Completed tasks. Record of your life activities. Rate of completion is your "velocity".
	from backlog.	 Key: Work is pulled. You are in charge! 	

Notes:

- Ready column is not strictly required, sometimes called "Selected for development".
- Other common column: In Review
- Can be creative with columns:
 - Waiting on Advisor Confirmation.
 - Blocked





Kanban principles

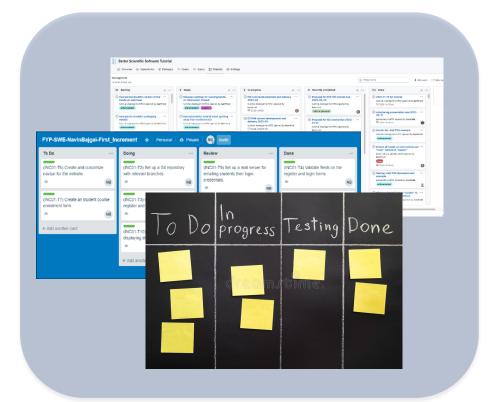
- Limit number of "In Progress" tasks
 - Must be tuned by each team
 - Common convention: 2n-1 tasks where n = # team members
- Productivity improvement:
 - Optimize "flexibility vs swap overhead" balance. No overcommitting.
 - Productivity weakness exposed as bottleneck. Team must identify and fix the bottleneck.
 - Effective in R&D setting. Avoids a deadline-based approach. Deadlines are dealt with in a different way.
- Provides a board for viewing and managing issues





Kanban tools

- Wall, whiteboard, blackboard: Basic approach.
- Software, cloud-based:
 - Trello, JIRA, GitHub or GitLab Issues & Project Boards
 - Many more.
- Trello (browser, Android, iPhone, iPad).
 - Can add, view, update, anytime, anywhere.
 - Different boards for different contexts
 - Effective when people are split on multiple projects







Big question: How many tasks?

- No single answer. Choose something and adjust from there.
- Personal Kanban approach: Start with 2 or 3.
- Use a freeway traffic analogy:
 - Does traffic flow best when fully packed? No.
 - Same thing with your effectiveness.
- Spend time consulting board regularly.
 - Brings focus.
 - Enables reflection, retrospection.
 - Use slack time effectively.
 - When you get out of the habit, start up again.
 - Steers towards previously started tasks





Code Review – What Peer Code Review Can Provide

- Allows discussion of proposed changes
 - Iterations for better code
 - Discussions and reviewing allow more understanding of the code
- Ensures requested change/feature met
- Evaluates impact of the change
 - Breakages
 - Interactions with other parts of code
- Ensures coding guidelines are met
- Improves practices by learning
 - About other parts of the code
 - Helpful coding techniques by others

Blog: How to code review in a Pull Request

Author: Hugo Sousa - March 17, 2021

https://blog.codacy.com/how-to-code-review-in-a-pull-request/





Code Review - Improvement and Practices

- Helpful practices for scientific research software
 - Make code review process formal with structured guidelines
 - Allocate sufficient time in the development process to perform code review
 - Try to ensure at least one science review and one technical review
 - Timely reviews provide quick feedback to incoming review requests
 - Train reviewers on how to phrase good feedback
 - Train developers to accept comments to improve their code
 - Include automatic code review tool and train reviewers in best use practice of the tool

Investing in Code Reviews for Better Research Software (2022-10-12)

Presenters: Thibault Lestang, Dominik Krzemiński and Valerio Maggio

https://ideas-productivity.org/events/hpc-best-practices-webinars/#webinar068

Testing and Code Review Practices in Research Software Development (2020-09-09)

Presenter: Nasir Eisty

https://ideas-productivity.org/events/hpc-best-practices-webinars/#webinar044





Software Licensing

- Any software you write is "born copyrighted"
 - Copyright holder is usually you (as author) or your employer (more likely)
- By default, that copyright is "all rights reserved" to the holder of the copyright
- Specifying a license controls how others can use or contribute to the software
 - Treat the license as a tool to help you accomplish your goals for the software
 - Potentially many considerations in choosing a license
- For open source licenses
 - Choose an Open Source Initiative approved license (don't make up your own)
 - Try a tool like https://choosealicense.com/
- Make sure your chosen license is clearly expressed in your code repository
- For a lot more info see: <u>Introduction to Software Licensing</u> from Best Practices for HPC Software Developers webinar series

Extra Slides – Git Workflows from CSE projects





Current Trilinos Workflow

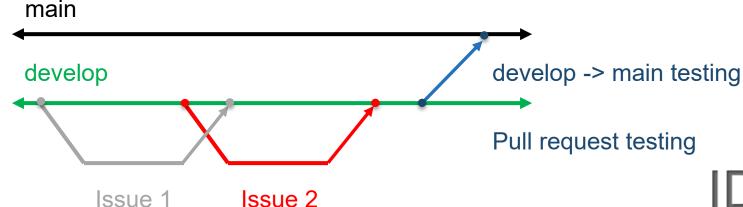
https://trilinos.github.io/

Test-driven workflow

- Feature branches start and end with develop
- All changes to develop must come from GitHub pull requests
- Feature branches are merged into develop only after passing pull request test suite
- Change sets from develop are tested daily for integration into main

Workflow designed so that

- All commits in main are in develop
- Merge conflicts exposed when integrating into develop
- Merge conflicts never occur when promoting to main







Current Open MPI Workflow

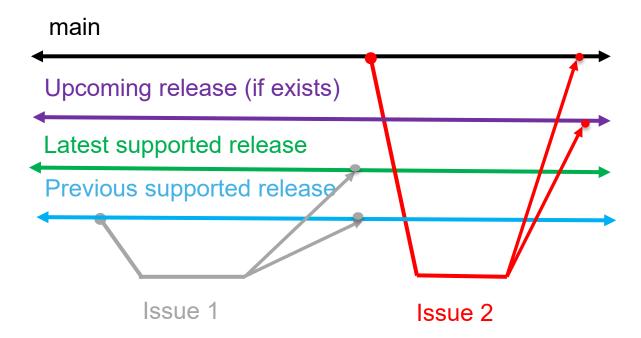
https://www.open-mpi.org

Versioning:

Major versions - break compatibility

Minor versions – visible

Releases correct issues



Workflow designed so that

- Support two most recent releases
- Issues are addressed on all applicable branches
- All PR's reviewed by at least one core developer
- Main and supported branches work at all times
- Developers work on main or feature branches depending on complexity of the changes

Testing

- CI testing on PR's for any branch using Jenkins (limited set of compilers, hardware, tests)
- Nightly testing on all branches using communitybuilt MTT framework (more complex set of compilers, hardware, tests)
- Additional testing for release candidates





devel non-backwards compatible new features go here 1.0 release branch only bug fixes go here (created at feature tag--1.0.0 1.1 release branch only bug fixes go here tag-1.1.1 v1 is in maintenance mode/we will not release 1.2, so merge changes back and start a 2.x branch new features

Current FleCSI Workflow

https://flecsi.github.io/flecsi

Versioning:

Incompatible - devel branch breaks compatibility with previous versions

Feature (1, 2 ...) named for major version

Release - (1.x, 2.x ...) named for major.minor version, correct issues, tags used for bug fixes.

Workflow designed so that

- All supported branches work at all times
- Merge Requests are tested and reviewed

Testing

- Customized unit-testing framework based on Google Test
- Special gitlab-ci branch images and configuration files





