

# LAMMPS Software Development on GitHub

Richard Berger  
Anders Hafreager

LAMMPS Workshop 2017

August 1, 2017

# LAMMPS GitHub Tutorial

## Target Audience

- ▶ LAMMPS Developers
- ▶ Package Maintainers
- ▶ Contributors

## Agenda

1. GitHub Workflow Overview
2. Git Introduction
3. Hands-on

# Outline

Background

Releases

Issue Tracking

Pull Requests

# Some History

## LAMMPS started as Fortran; rewritten in C++

- ▶ make it easy to add new kernels (“styles”)
- ▶ implemented as derived polymorph classes
- ▶ top-level code is an instance of a composite of instances of selected styles/classes

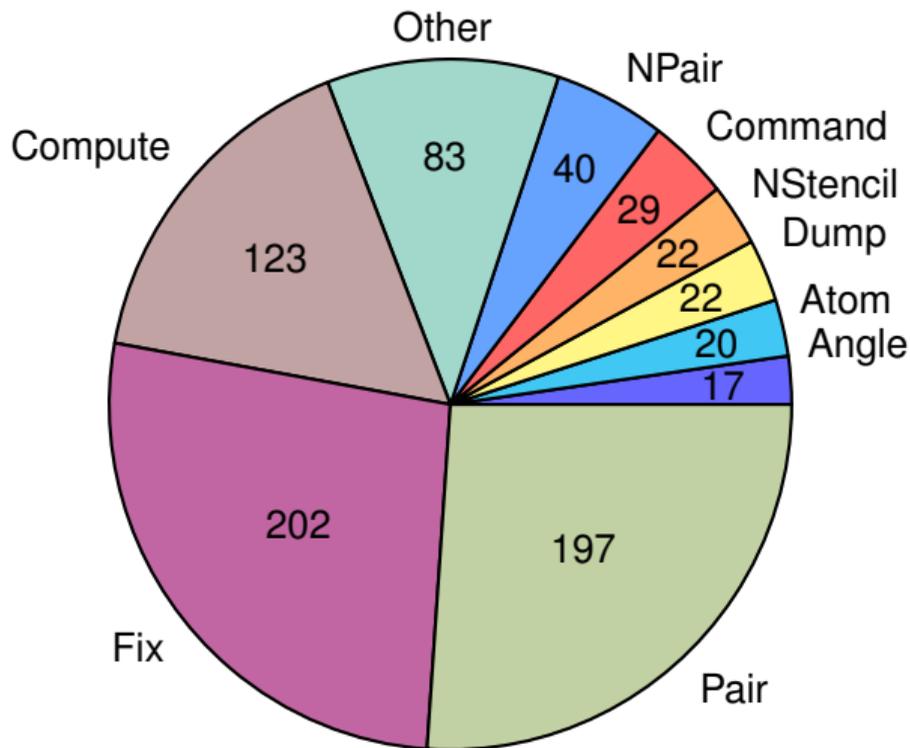
## Linear development

- ▶ originally not using any dedicated source code management tools
- ▶ later adapted Subversion for version control

## Continuous development model

- ▶ changes released quickly and frequently
- ▶ core code was supposed to always work

## LAMMPS in numbers



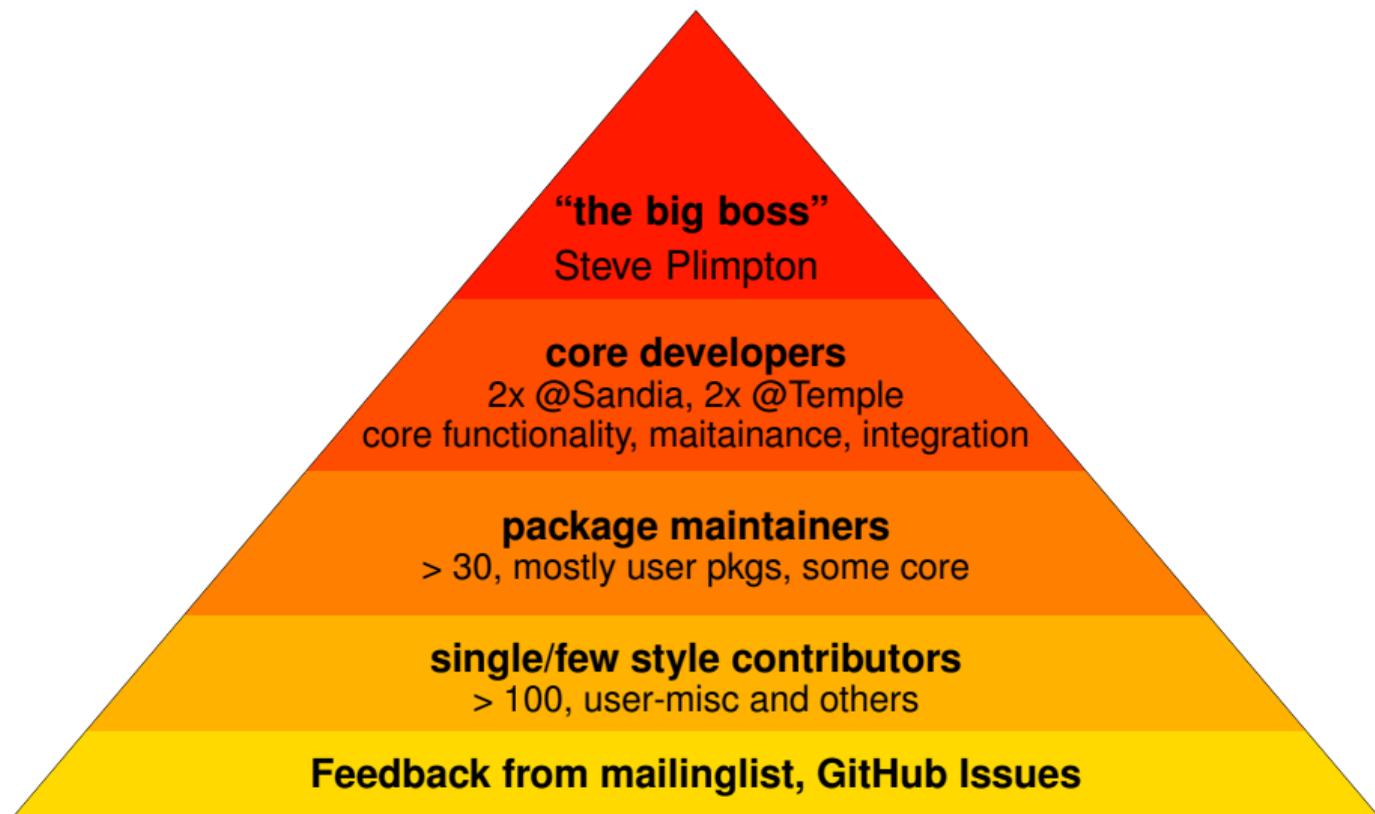
- ▶ 750+ styles (1250+ if you count accelerator variants)
- ▶ 31 packages
- ▶ 30 USER packages
- ▶ 21 external libraries
- ▶ One dozen features enabled through compiler flags (e.g.
  - DLAMMPS\_PNG,
  - DLAMMPS\_FFMPEG)

## Commit History in the old workflow

Release Tag	Date	Commits	Authors
r15407	305	2016-07-30	<b>sjplimp (289)</b> , athomps (11), stamoor (5)
r15061	369	2016-05-17	<b>sjplimp (329)</b> , stamoor (26), athomps (14)
r14624	261	2016-02-15	<b>sjplimp (222)</b> , stamoor (24), athomps (15)
r14304	368	2015-12-08	<b>sjplimp (286)</b> , athomps (71), stamoor (11)
r13864	282	2015-08-10	<b>sjplimp (245)</b> , athomps (25), stamoor (12)
r13475	319	2015-05-15	<b>sjplimp (290)</b> , athomps (14), pscrozi (8), stamoor (7)

- ▶ Attributions would go into README files and [lammeps.sandia.gov/authors.html](http://lammeps.sandia.gov/authors.html)
- ▶ Contributions and Integration work not visible

# LAMMPS Development Pyramid



# Why change the workflow?

continuing growth increases maintenance effort

accelerated styles increase code complexity

base class changes may break derived classes

disruptive changes to core may need contributions from multiple developers

need a facility for **concurrent** development and open/reviewable communication between contributors/maintainers

offload some code integration to contributor

provide feedback on merging effort



- ▶ distributed version control system
- ▶ efficient handling of feature branches
- ▶ powerful merging tool



- ▶ public and well performing git hosting
- ▶ also communication platform: discussions tied to issues or pull requests
- ▶ provides API and triggers for testing tasks



## Jenkins

- ▶ continuous integration and testing platform
- ▶ allows us to define compilation and testing pipelines
- ▶ operates on multiple platforms

# Workflow Documentation

- ▶  **LAMMPS Contributing Guidelines**

<https://github.com/lammps/lammps/blob/master/.github/CONTRIBUTING.md>

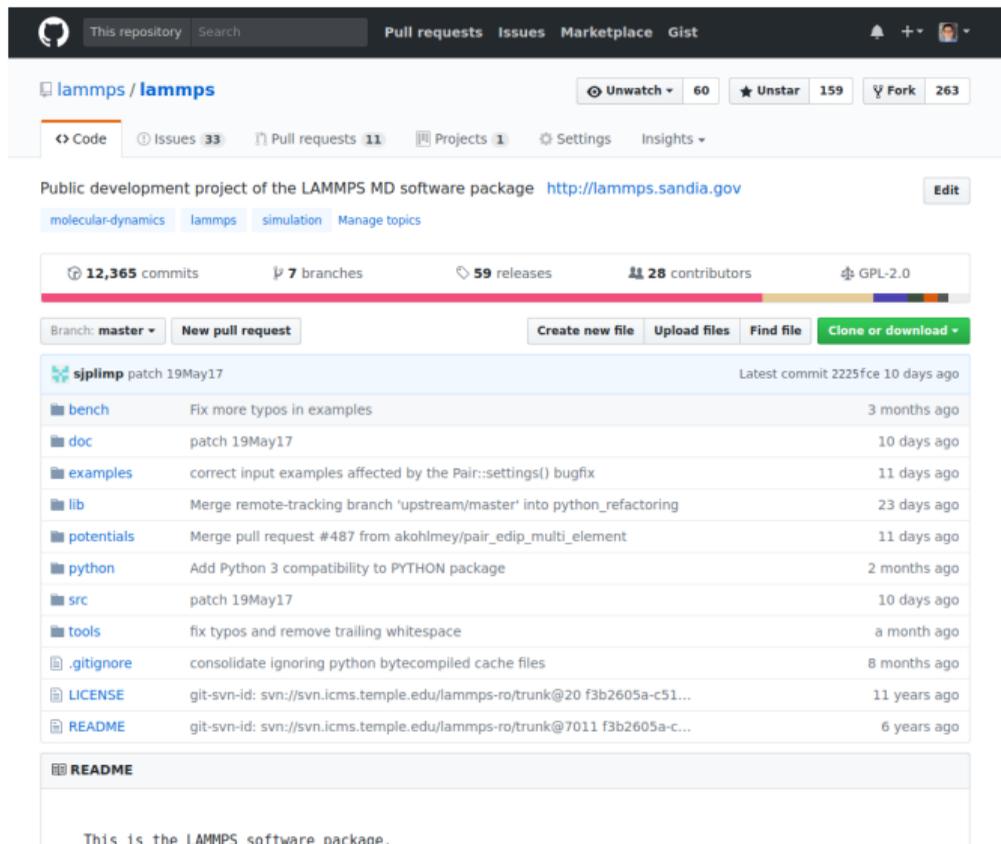
- ▶  **LAMMPS GitHub Tutorial**

[http://lammps.sandia.gov/doc/tutorial\\_github.html](http://lammps.sandia.gov/doc/tutorial_github.html)

## Note

These are best practises which developed over time. They're not set in stone and we continue to improve it.

# LAMMPS on GitHub



This repository Search Pull requests Issues Marketplace Gist

lammps / lammps Unwatch 60 Unstar 159 Fork 263

Code Issues 33 Pull requests 11 Projects 1 Settings Insights

Public development project of the LAMMPS MD software package <http://lammps.sandia.gov> Edit

molecular-dynamics lammps simulation Manage topics

12,365 commits 7 branches 59 releases 28 contributors GPL-2.0

Branch: master New pull request Create new file Upload files Find file Clone or download

sjplimp patch 19May17 Latest commit 2225fce 10 days ago

bench	Fix more typos in examples	3 months ago
doc	patch 19May17	10 days ago
examples	correct input examples affected by the Pair::settings() bugfix	11 days ago
lib	Merge remote-tracking branch 'upstream/master' into python_refactoring	23 days ago
potentials	Merge pull request #487 from akohlmeij/pair_edip_multi_element	11 days ago
python	Add Python 3 compatibility to PYTHON package	2 months ago
src	patch 19May17	10 days ago
tools	fix typos and remove trailing whitespace	a month ago
.gitignore	consolidate ignoring python bytecompiled cache files	8 months ago
LICENSE	git-svn-id: svn://svn.icms.temple.edu/lammps-ro/trunk@20 f3b2605a-c51...	11 years ago
README	git-svn-id: svn://svn.icms.temple.edu/lammps-ro/trunk@7011 f3b2605a-c...	6 years ago

README

This is the LAMMPS software package.

🌐 <http://github.com/lammps/lammps>

- ▶ public development repository
- ▶ issue tracking
- ▶ changes from Sandia SVN are integrated here before new releases
- ▶ contributions are processed as Pull Requests for **code review** and **testing**

# Release Policy

## Patch Releases

- ▶ a collection of bugfixes and new features
- ▶ every few weeks
- ▶ posted on website as tarball

## Stable Releases

- ▶ a release marked as stable after longer periods of testing
- ▶ derived from latest patch release
- ▶ period of feature-freeze and only accepting bugfixes
- ▶ released about every 3-4 months
- ▶ posted on website as tarball

# Public Development on GitHub

## master branch

- ▶ main development branch
- ▶ the latest and greatest development version of LAMMPS
- ▶ while we try really hard to keep it stable, things might break for brief periods of time
- ▶ even changes from Sandia are integrated back by Steve to GitHub via Pull Requests

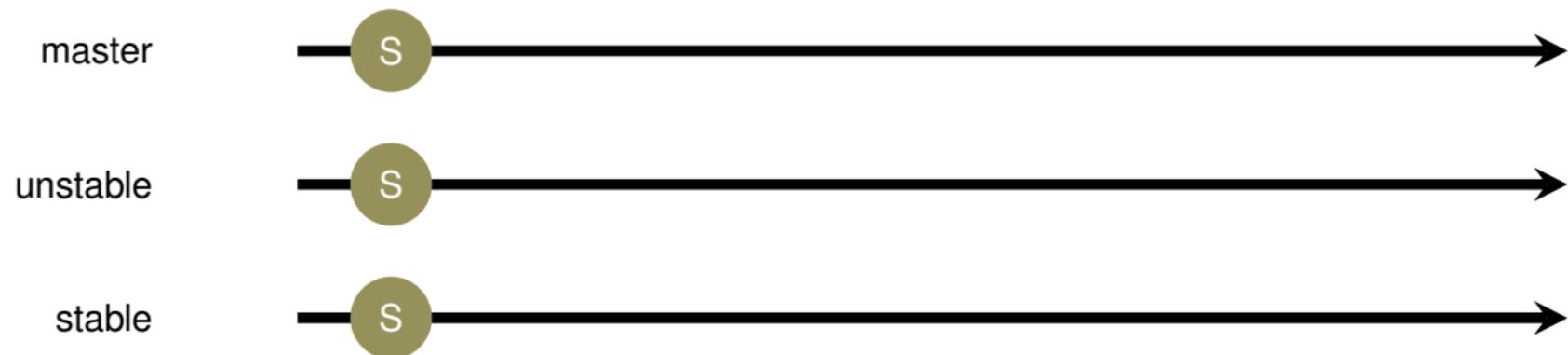
## unstable branch

- ▶ a bit older than **master**
- ▶ follows patch releases

## stable branch

- ▶ a bit older than **unstable**
- ▶ follows stable releases

# LAMMPS Branches



change

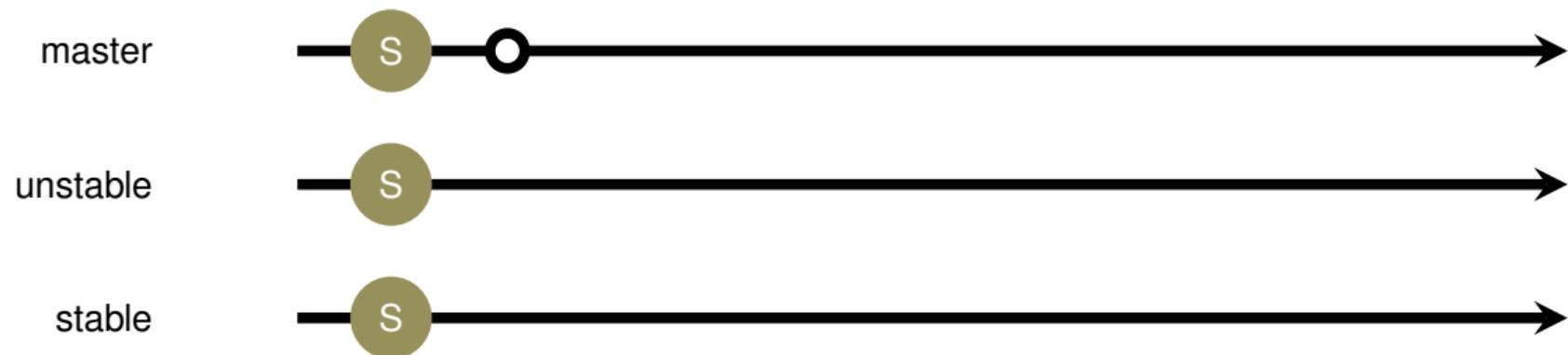


patch release



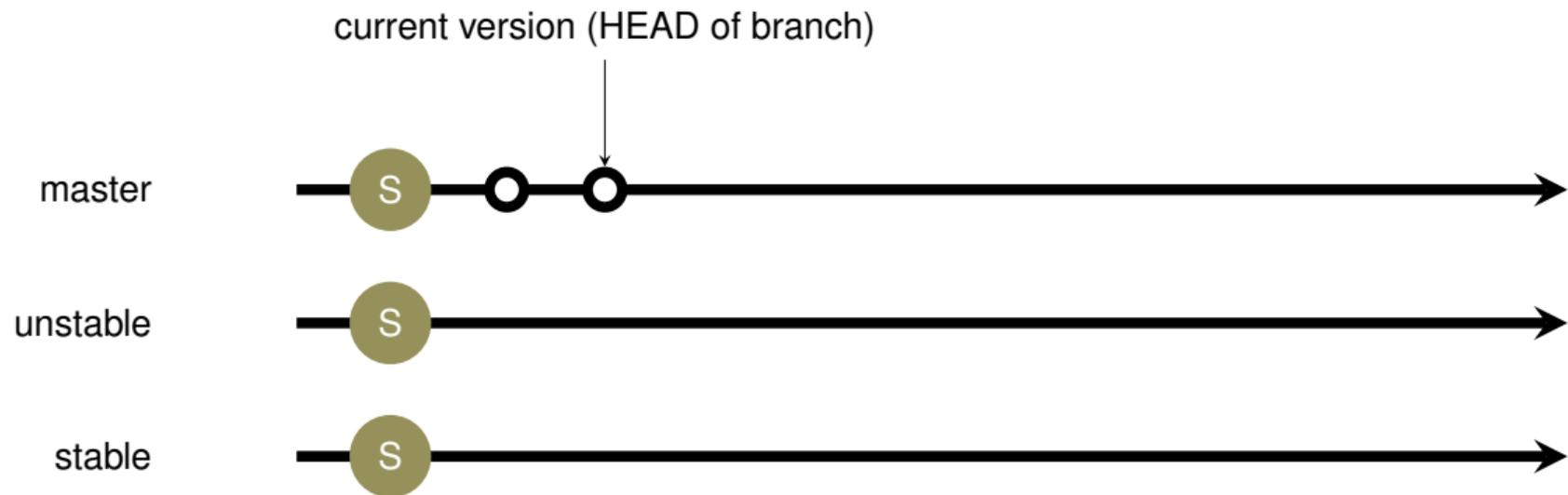
stable release

# LAMMPS Branches



-  change
-  patch release
-  stable release

# LAMMPS Branches



change

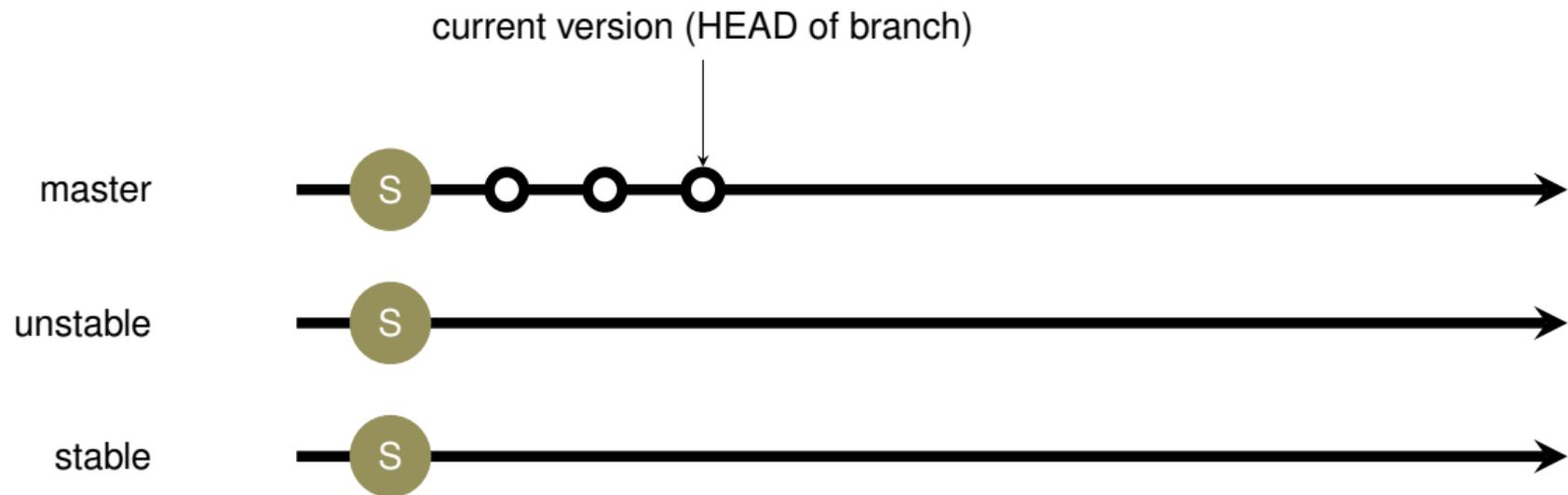


patch release



stable release

# LAMMPS Branches

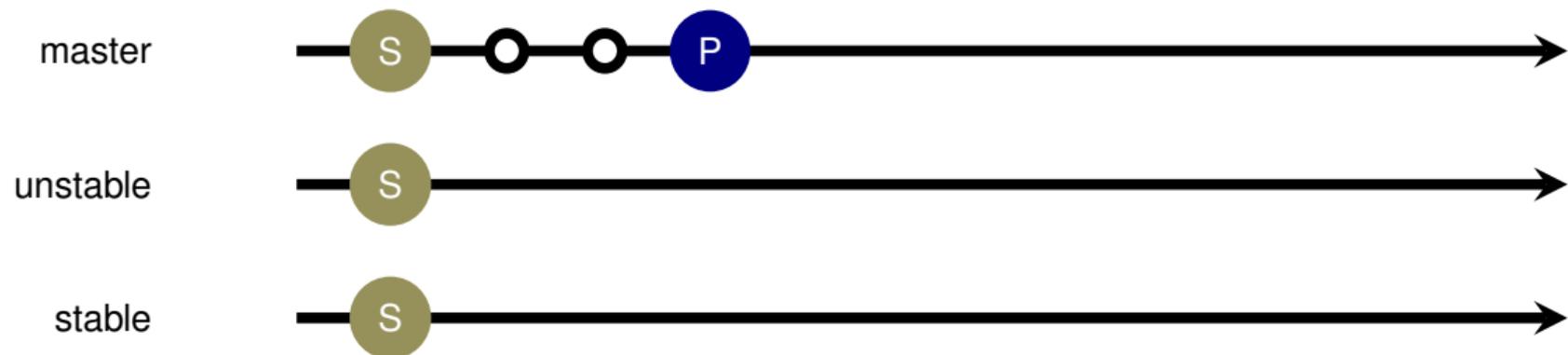


○ change

● P patch release

● S stable release

# LAMMPS Branches



change

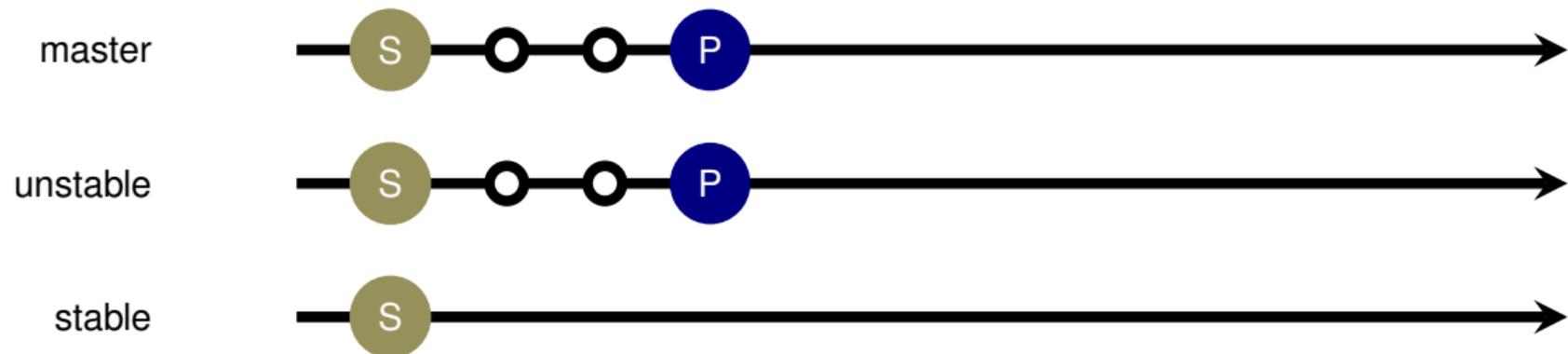


patch release



stable release

# LAMMPS Branches



change

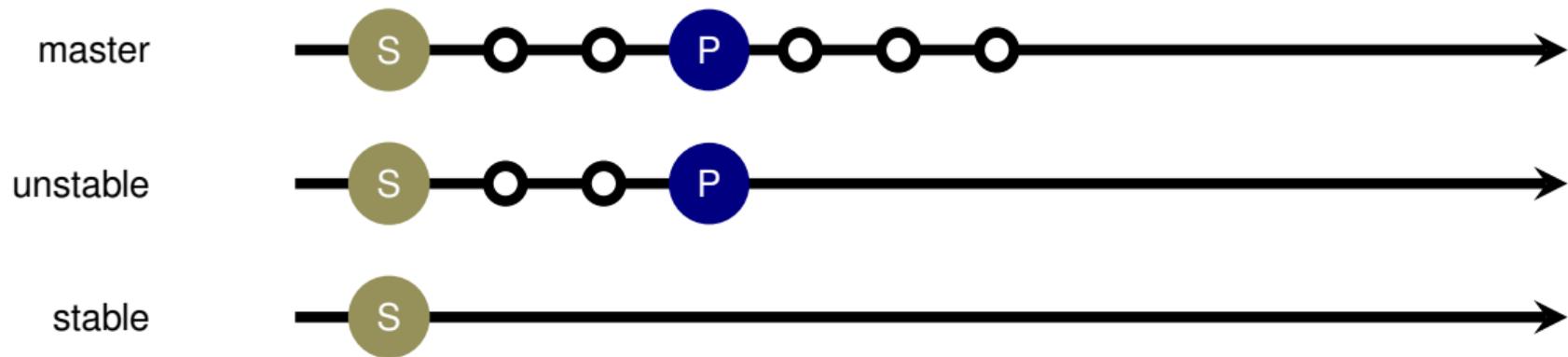


patch release



stable release

# LAMMPS Branches



change

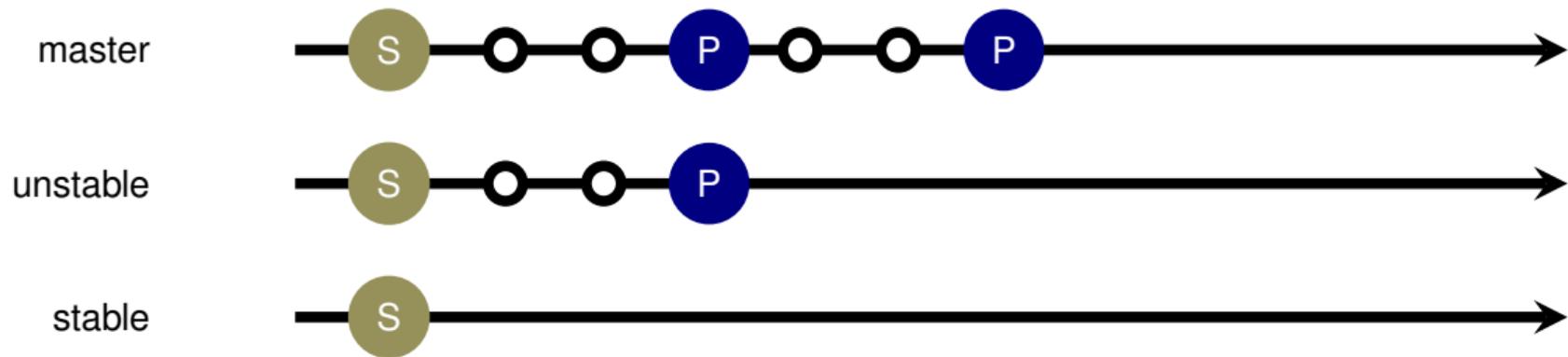


patch release



stable release

# LAMMPS Branches



change

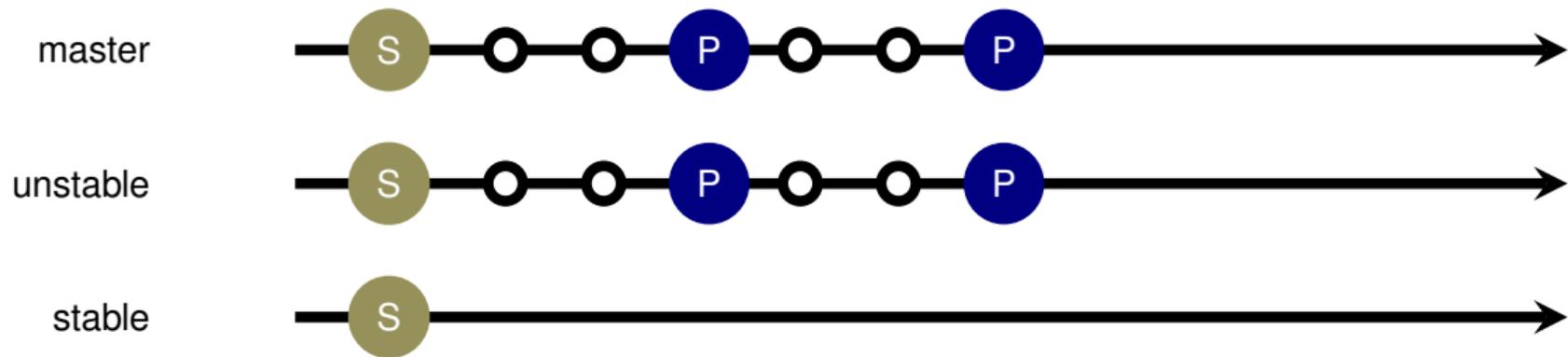


patch release



stable release

# LAMMPS Branches



change

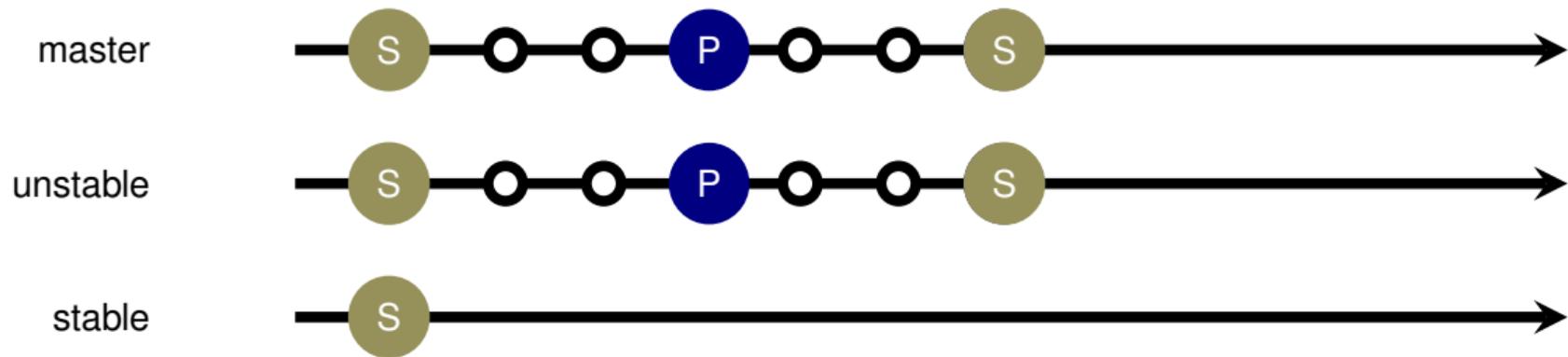


patch release



stable release

# LAMMPS Branches



change

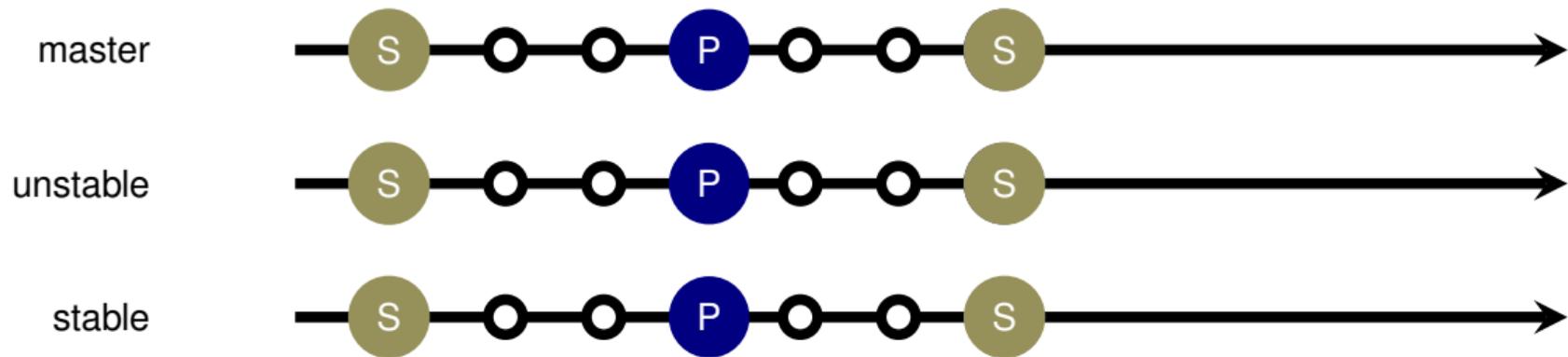


patch release



stable release

# LAMMPS Branches



change

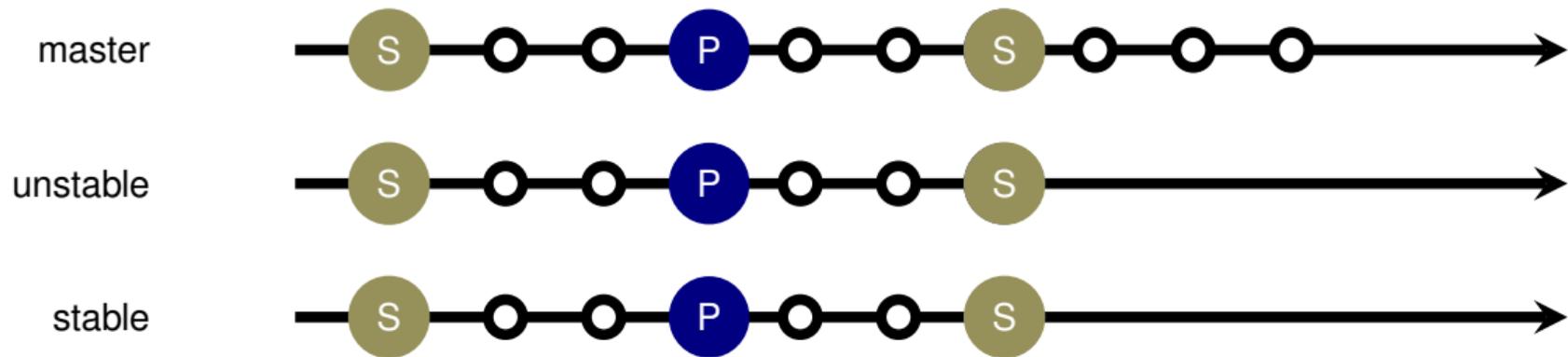


patch release



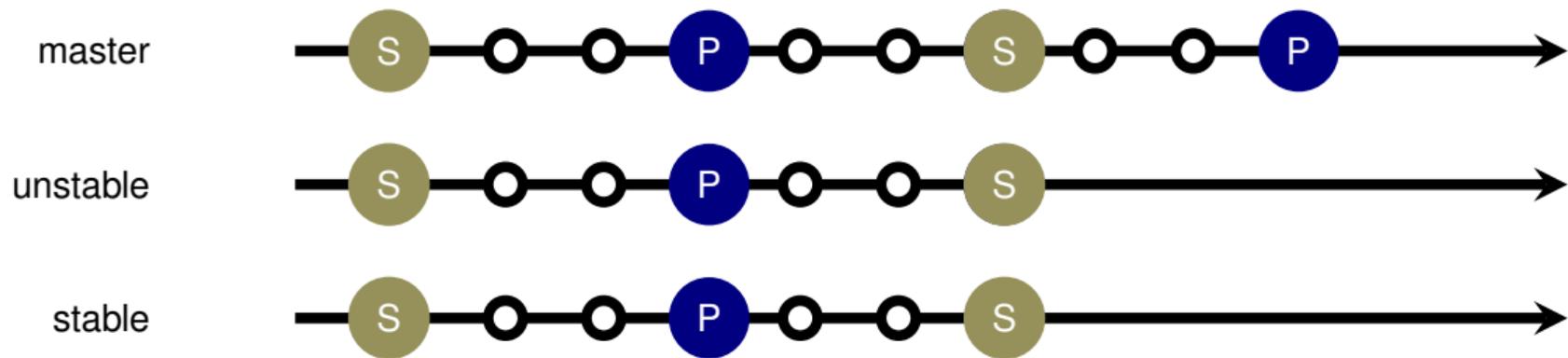
stable release

# LAMMPS Branches



-  change
-  patch release
-  stable release

# LAMMPS Branches



change

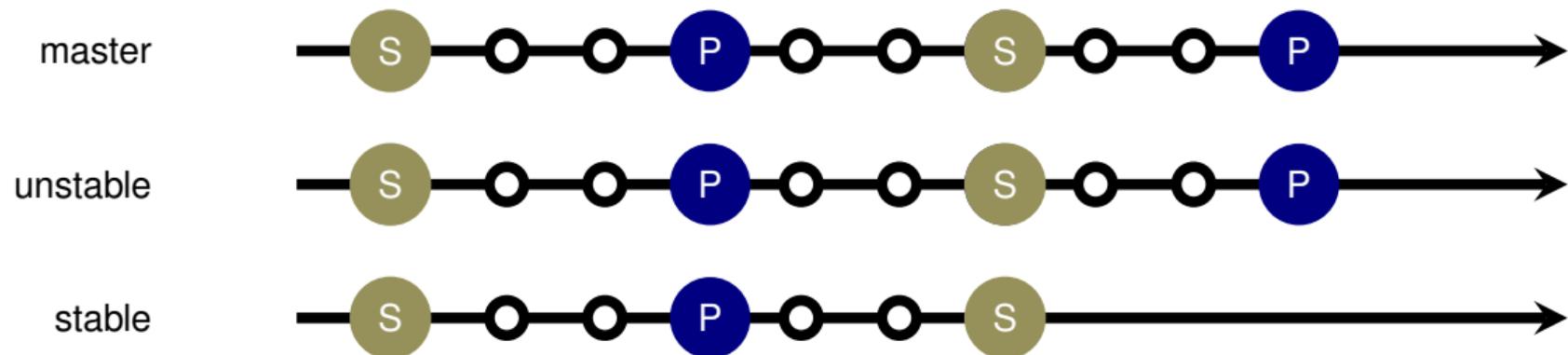


patch release

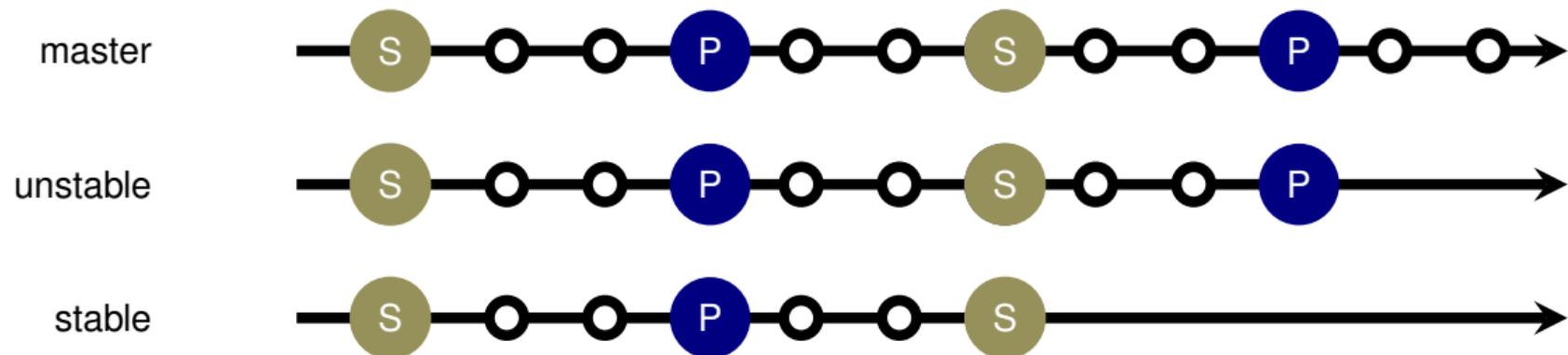


stable release

# LAMMPS Branches



# LAMMPS Branches



# Releases on GitHub

 [Features](#) [Business](#) [Explore](#) [Marketplace](#) [Pricing](#) This repository  [Sign in](#) or [Sign up](#)

[lammps / lammps](#) Watch 60 Star 187 Fork 285

[Code](#) [Issues 30](#) [Pull requests 8](#) [Insights](#)

[Releases](#) [Tags](#)

Since 6 days ago Show 8 newer tags

Latest release  
[stable\\_31Mar2017](#)  
[ae56b9a](#)

## LAMMPS stable release 31 Mar 2017

 **akohlmeys** released this on Mar 30 · 659 commits to master since this release

Notable new features in this release are:

- refactoring of the neighbor list construction to be more modular and extensible from packages. active neighbor list modules are reported in the output
- updates, performance improvements and new styles for the `KOKKOS` and `USER-INTEL` packages
- bugfixes and refactoring of parts of `AIREBO` and `AIREBO-M` addressing some of the occasionally observed instabilities with the LAMMPS implementation



# Releases on GitHub

## Downloads

 [Source code](#) (zip)

 [Source code](#) (tar.gz)

on Mar 30

**patch\_31Mar2017** 

 [ae56b9a](#)  [zip](#)  [tar.gz](#)

Previous

Next

# Releases on GitHub

[Features](#)[Business](#)[Explore](#)[Marketplace](#)[Pricing](#)[This repository](#)[Sign in](#) or [Sign up](#)[lammps](#) / **lammps**[Watch](#)

60

[★ Star](#)

187

[Fork](#)

285

[Code](#)[Issues](#) 30[Pull requests](#) 8[Insights](#) ▾[Releases](#)[Tags](#)

6 days ago

**patch\_24Jul2017** ...[a59b7e4](#) [zip](#) [tar.gz](#)

24 days ago

**patch\_6Jul2017** ...[4339379](#) [zip](#) [tar.gz](#)

on Jun 23

**patch\_23Jun2017** ...[1370385](#) [zip](#) [tar.gz](#)

on Jun 20

**patch\_20Jun2017** ...[87c028e](#) [zip](#) [tar.gz](#)

on May 19

**patch\_19May2017** ...[2225fce](#) [zip](#) [tar.gz](#)

on May 4

**patch\_4May2017** ...

# Issue tracking

## Usage:

- ▶ tracking bugs
- ▶ feature requests
- ▶ planning new features

## Labels

- ▶ applied by maintainers
- ▶ used to group by topic

## Assignment

- ▶ One or more contributors
- ▶ Meaning: ownership and responsible for resolution

The screenshot shows a GitHub issue page for the repository 'lammps / lammps'. The issue title is 'Implement short neighborlists on manybody potentials in GPU package #543'. It was opened by 'andeplane' on June 22 and has 3 comments. The issue is currently open. The main content of the issue is a comment from 'andeplane' dated June 22, which discusses the implementation of short neighborlists in the GPU package, comparing CPU and KOKKOS versions and mentioning the use of vashishta, sw, and tersoff. The comment also mentions that the GPU package is nice because it supports single/mixed precision and works in Atomify. A comment from 'stanmoore1' dated June 26 indicates that labels 'bugfix', 'enhancement', and 'gpu\_package' were added, and 'bugfix' was removed. Another comment from 'andeplane' dated 26 days ago mentions contact with '@ndtrung81' and 'Mike' regarding the issue. A comment from 'stanmoore1' dated 19 days ago says '@andeplane, glad to hear'. At the bottom, it shows that 'akohlmeiy' assigned 'andeplane' and 'ndtrung81' 17 days ago. The right sidebar shows the issue's metadata, including assignees ('andeplane', 'ndtrung81'), labels ('enhancement', 'gpu\_package'), projects (None yet), milestones (No milestone), and notifications (Unsubscribe button). There are also 3 participants listed.



# Implement short neighborlists on manybody potentials in GPU package #543

Edit

New issue

**Open** andeplane opened this issue on Jun 22 · 3 comments

andeplane commented on Jun 22

Collaborator + 👤 ✎

In CPU and KOKKOS versions of vashishta, sw and tersoff, we use short neighbor lists that only contains neighbors within cutoff. This is especially useful in vashishta where 3-body forces usually have much smaller cutoff.

The GPU package is nice since it supports single/mixed precision and works in Atomify, so I'm interested in porting this feature into the GPU package as well. I'm not so familiar with how it actually does neighbor list building etc, so if anyone knows how to do this easily, feel free to do it :D If not I'll probably try to understand how it's done.



stanmoore1 added **bugfix** **enhancement** **gpu\_package** and removed **bugfix** labels on Jun 26



andeplane commented 26 days ago

Collaborator + 👤 ✎ ✕

I have been in contact with @ndtrung81 and Mike on email about this. I think I know how to do it and will get help on the way. Probably done within a month or two.



stanmoore1 commented 19 days ago

Member + 👤 ✎ ✕

@andeplane, glad to hear

## Assignees



andeplane  
ndtrung81

## Labels



enhancement  
gpu\_package

## Projects



None yet

## Milestone



No milestone

## Notifications

Unsubscribe

You're receiving notifications because you're subscribed to this repository.

3 participants

# Writing issue descriptions and comments: Markdown Syntax

## Headers

```
# Header 1  
## Header 2  
### Header 3
```

## Ordered Lists

1. first
2. second
3. third

## Code Snippets

```
```language  
code  
```
```

## Unordered Lists

- \* first
- \* second
- \* third

## Links

```
[Link] (http://www.google.com)
```

# Writing issue descriptions and comments: Markdown Syntax

## Task list with check boxes

```
* [ ] Task A
* [x] Task B
* [ ] Task C
```

## Images and Attachments

- ▶ Each comment can add images or files (certain types). Simply drag & drop them into the editor.

## Mention other users

By adding `@username` to your message, you create a reference to that user. They will also get notified of that comment. This is a way to direct the conversation in an issue or pull request.

## Not An Issue



- ▶ Issues are for code development related topics only!
- ▶ **Do not create an issue to ask how to use LAMMPS or discuss physics!**
- ▶ They will be ignored and closed. ⇒ Use the mailing list instead.

## Working on Code

- ▶ So you've assigned yourself to an issue and working on a fix
- ▶ Or you are implementing a new feature
- ▶ What now?

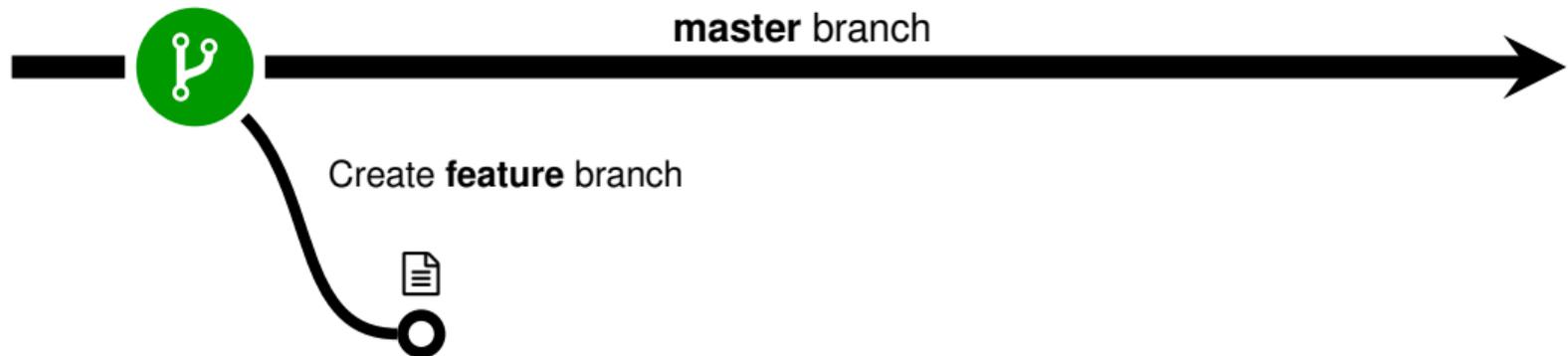
# Working on Code

- ▶ So you've assigned yourself to an issue and working on a fix
- ▶ Or you are implementing a new feature
- ▶ What now?

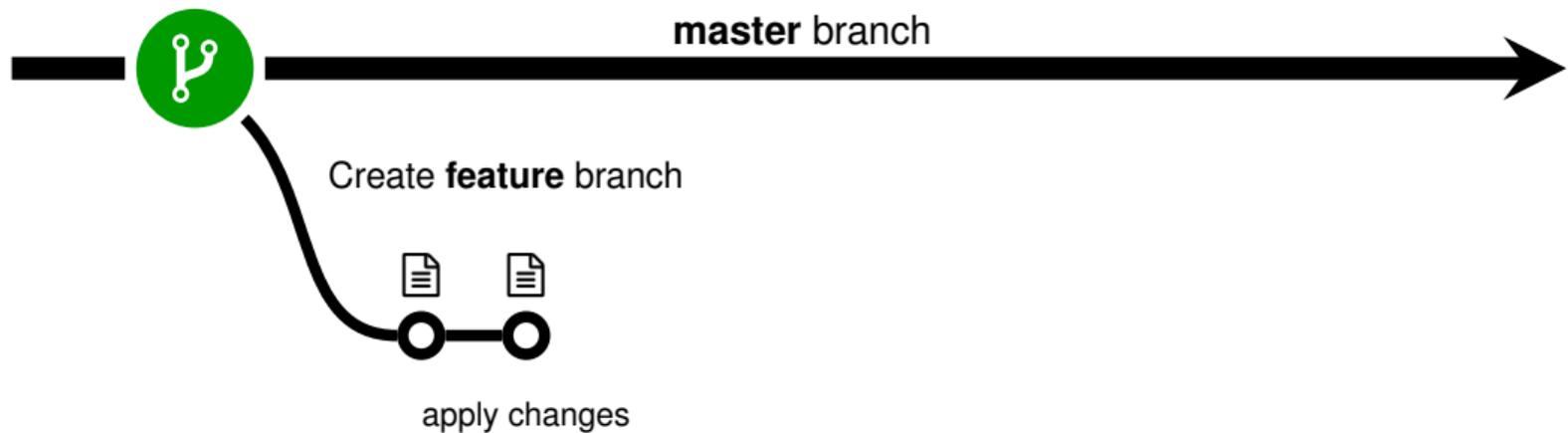
## GitHub Workflow

1. Get the latest code (master)
2. Create a git branch to work on
3. Save your changes in that branch
4. Create a pull request
5. Follow core developer's instructions and modify your contribution accordingly
6. Wait for merge

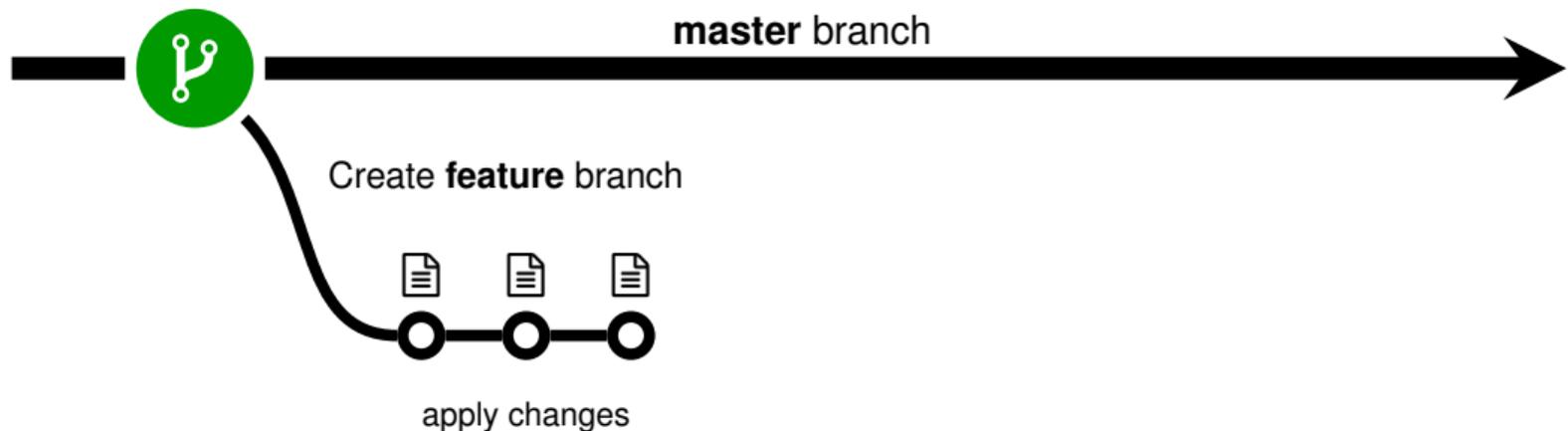
# GitHub Workflow



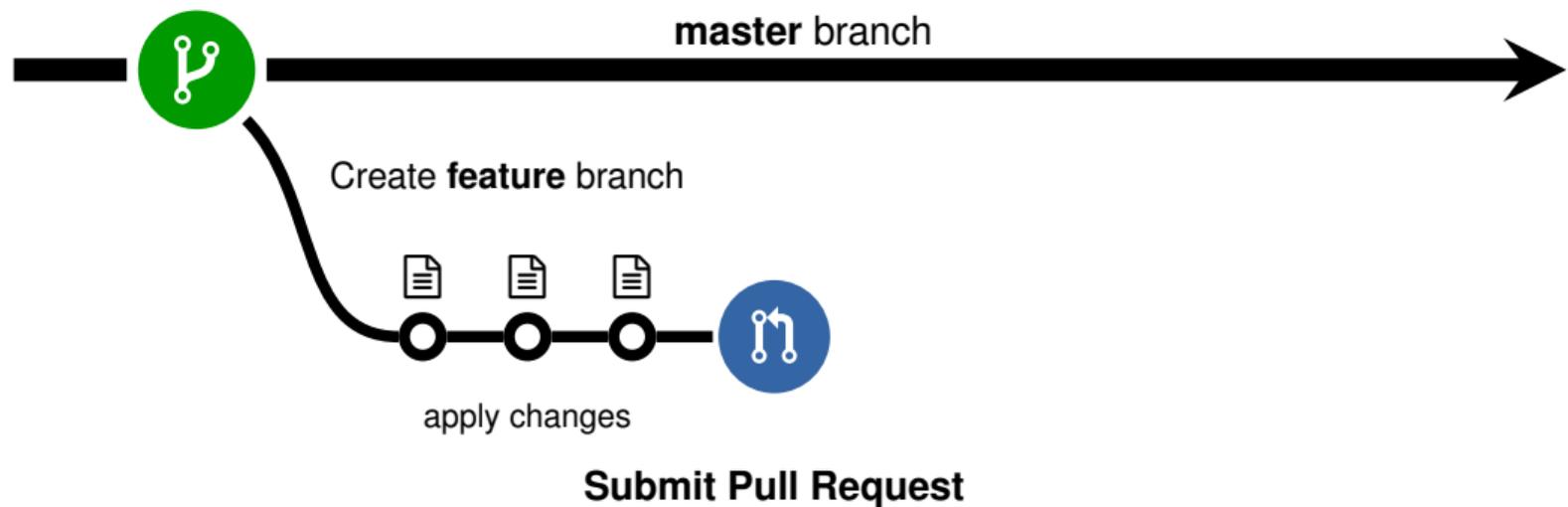
# GitHub Workflow



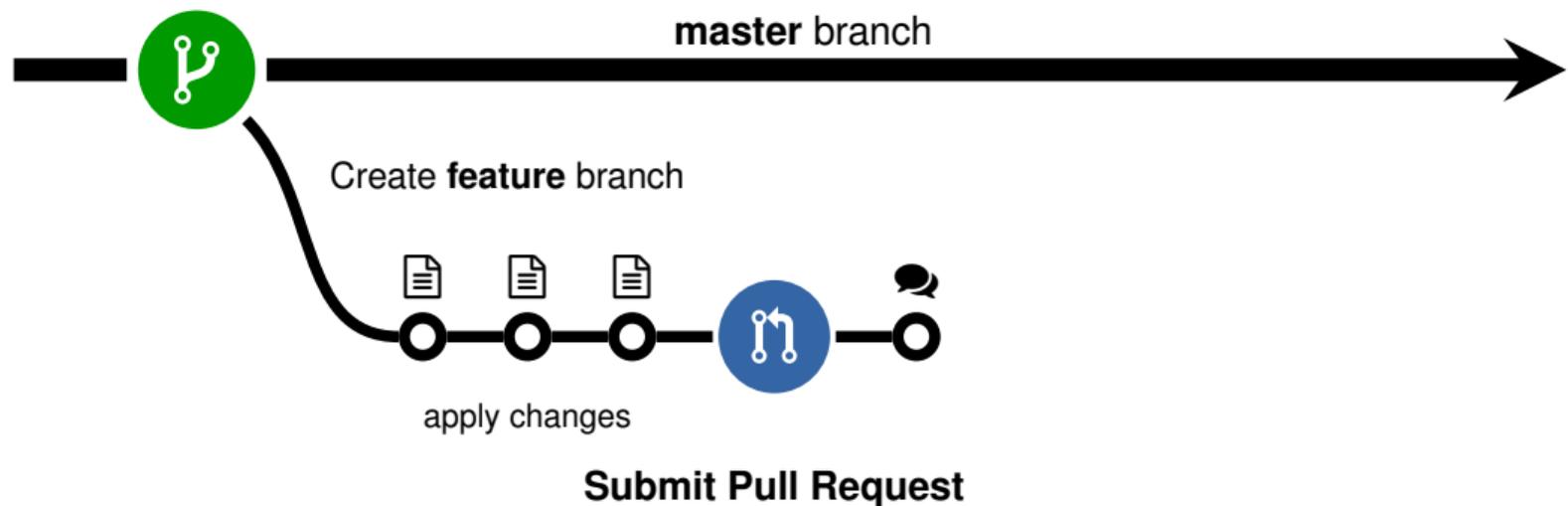
# GitHub Workflow



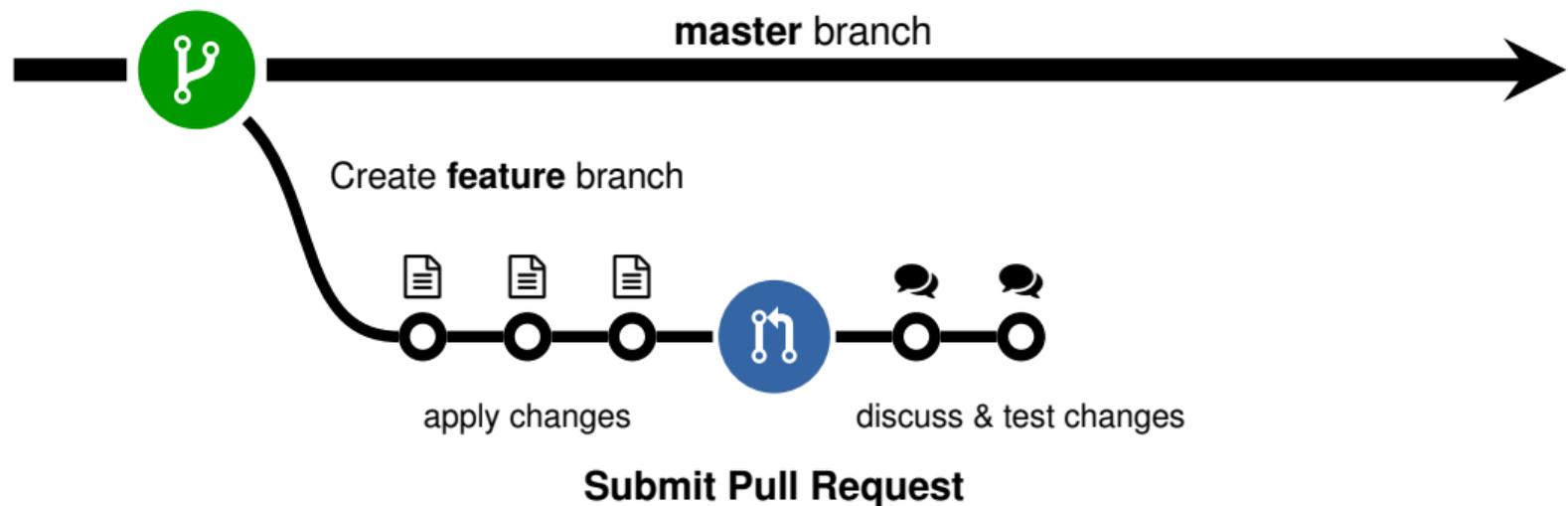
# GitHub Workflow



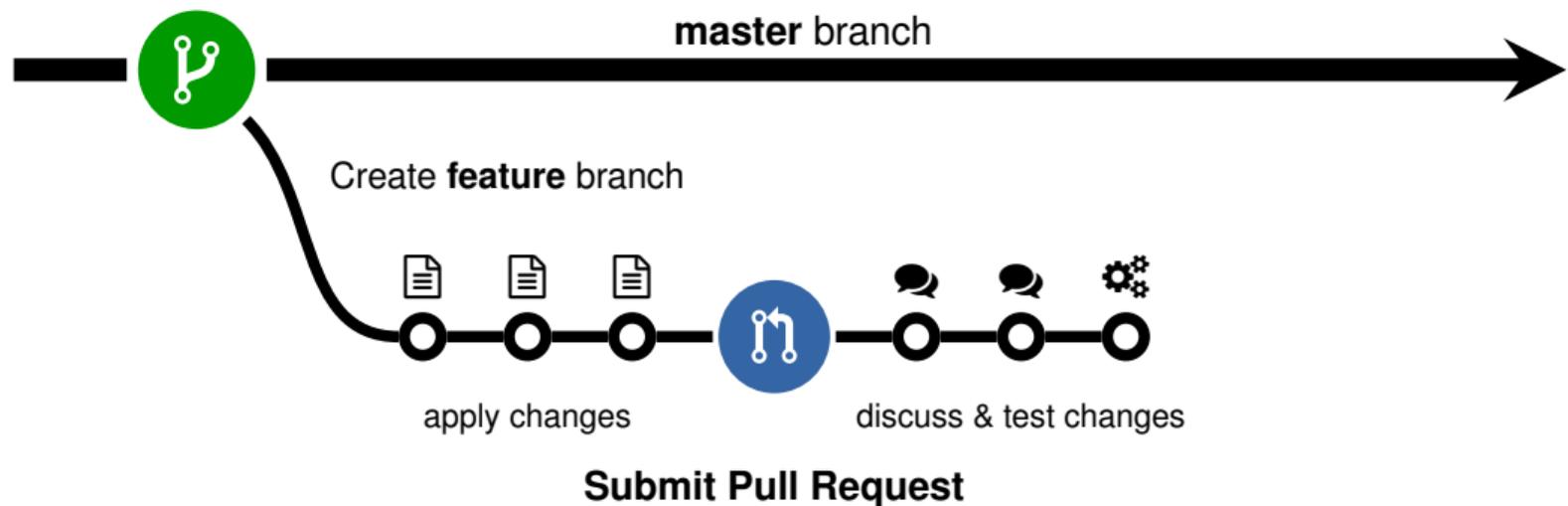
# GitHub Workflow



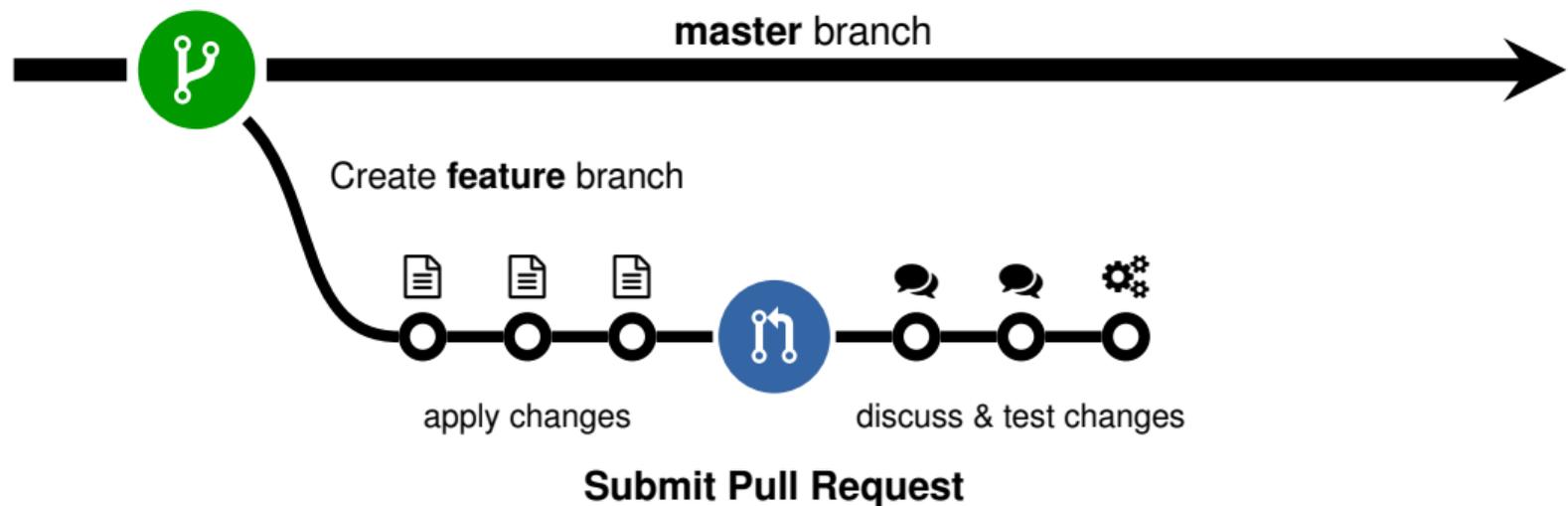
# GitHub Workflow



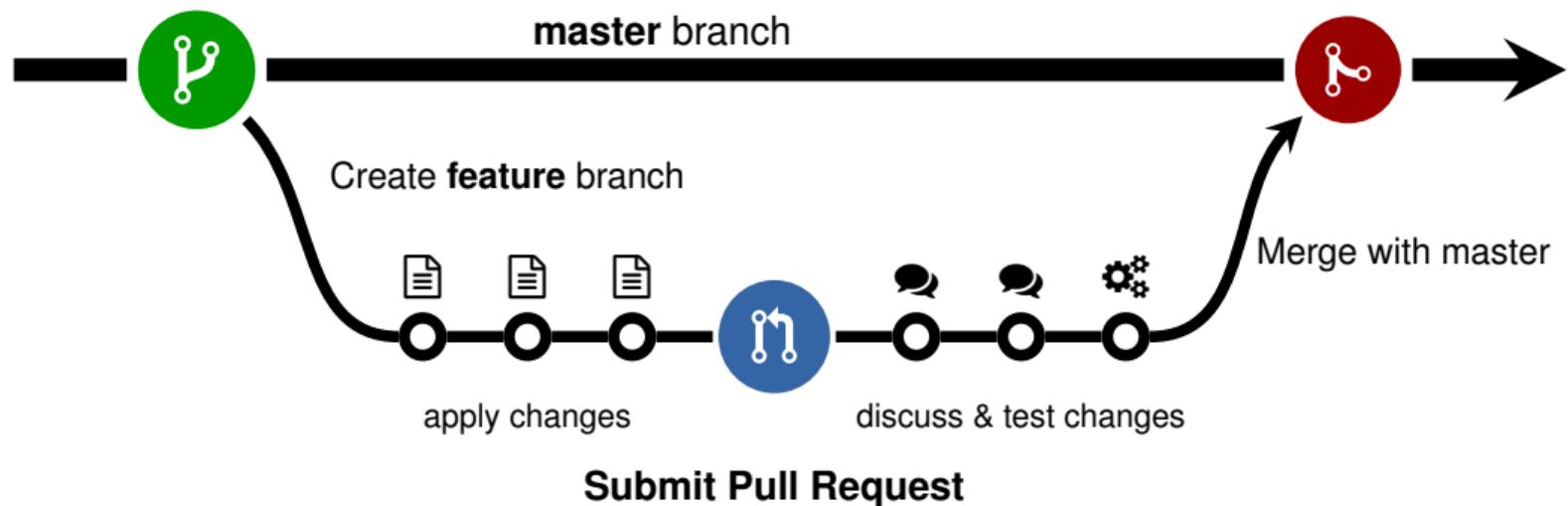
# GitHub Workflow



# GitHub Workflow



# GitHub Workflow



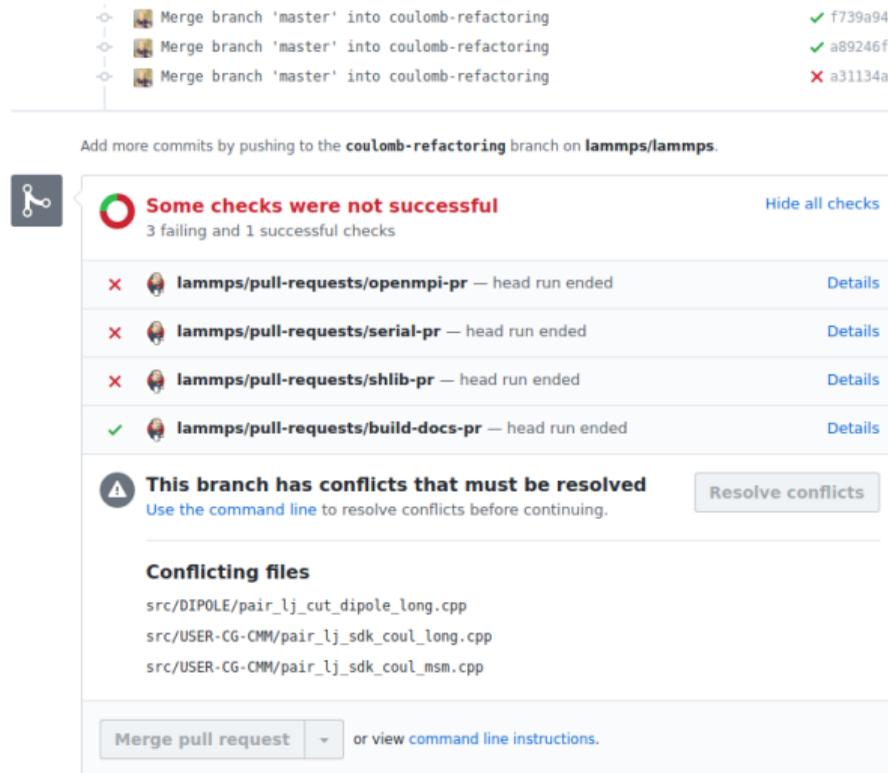
# Pull Requests: Contents

- ▶ a branch containing a sequence of changes
- ▶ summarized as the list of commits and files changed
- ▶ the goal is to combine this sequence of changes to the **master** branch
- ▶ like an issue, a PR can have a rich-text description
- ▶ For your convenience, any new pull request will start with a template text which you are supposed to fill out and edit accordingly

The screenshot shows a GitHub Pull Request (PR) page for the repository 'lammps / lammps'. The PR title is 'Implementing short neighbor lists for three-body gpu styles #597'. It is an 'Open' PR by user 'ndrung81' who wants to merge 10 commits into the 'lammps:master' branch from the 'ndrung81:three-body-short-nList' branch. The PR has 4 conversations, 10 commits, and 17 files changed. It has a net score of +1,168 and -905. The PR description includes a 'Purpose' section explaining that the PR closes #543 and adds support for short neighbor lists for kernels in 3-body /gpu styles (sw, tersoff\* and vashista). The 'Author(s)' section lists Trung D. Nguyen (Northwestern University) with thanks to Anders Hafreager (@andepiane). The 'Backward Compatibility' section states that the changes do not break backward compatibility. The 'Implementation Notes' section explains that in cases where the neighbor list is built on the device (neigh yes) or on the host with the number of threads per atom equal 1 (tpa 1), the 3-body gpu styles build a short neighbor list from the existing neighbor list data at every time step. The right sidebar shows the 'Reviewers' section with 'andepiane' as a reviewer, and the 'Assignees' section with 'ndrung81' as the assignee. The 'Labels' section shows 'enhancement' and 'gpu\_package' as labels. The 'Projects' section shows 'None yet'. The 'Milestone' section shows 'No milestone'. The 'Notifications' section shows an 'Unsubscribe' button. The bottom right corner features the 'LE UNIVERSITY' logo.

# Pull Requests: Automatic Testing

- ▶ Once a PR is submitted, your changes will be automatically tested
- ▶ Pushing further changes to your branch will be appended to the PR and be tested again
- ▶ Click “Details” to get to Jenkins



The screenshot displays a GitHub pull request interface. At the top, three merge actions are listed: 'Merge branch 'master' into coulomb-refactoring', each with a green checkmark and a commit hash (f739a94, a89246f, and a31134a). Below this, a message states: 'Add more commits by pushing to the coulomb-refactoring branch on lammps/lammps.' The main section features a 'Some checks were not successful' notification with a red circle icon, indicating '3 failing and 1 successful checks'. A 'Hide all checks' link is visible. The checks are listed as follows:

| Status | Job Name                           | Message          | Action  |
|--------|------------------------------------|------------------|---------|
| ✗      | lammps/pull-requests/openmpi-pr    | — head run ended | Details |
| ✗      | lammps/pull-requests/serial-pr     | — head run ended | Details |
| ✗      | lammps/pull-requests/shlib-pr      | — head run ended | Details |
| ✓      | lammps/pull-requests/build-docs-pr | — head run ended | Details |

Below the checks, a warning message states: 'This branch has conflicts that must be resolved'. It includes a 'Resolve conflicts' button and instructions: 'Use the command line to resolve conflicts before continuing.' The 'Conflicting files' section lists:

- src/DIPOLE/pair\_lj\_cut\_dipole\_long.cpp
- src/USER-CG-CMM/pair\_lj\_sdk\_coul\_long.cpp
- src/USER-CG-CMM/pair\_lj\_sdk\_coul\_msm.cpp

At the bottom, there is a 'Merge pull request' button and a link to 'view command line instructions.'

# Pull Requests: Automatic Testing - Jenkins

-  [Back to Project](#)
-  [Status](#)
-  [Changes](#)
-  [Console Output](#)
-  [View as plain text](#)
-  [View Build Information](#)
-  [GitHub PR Polling Log](#)
-  [Parameters](#)
-  [Open Blue Ocean](#)
-  [GNU Make + GNU C Compiler Warnings](#)
-  [Static Analysis Warnings](#)
-  [Embeddable Build Status](#)
-  [Previous Build](#)

## Build #928 (Jul 28, 2017 4:11:30 PM)

Started 2 days 1 hr ago  
Took [5 min 54 sec](#)



No changes.



GitHub PR [#600](#), Commit changed



This run spent:

- 8 sec waiting in the queue;
- 5 min 54 sec building on an executor;
- 6 min 2 sec total from scheduled to completion.



GNU Make + GNU C Compiler Warnings: [188 warnings](#).

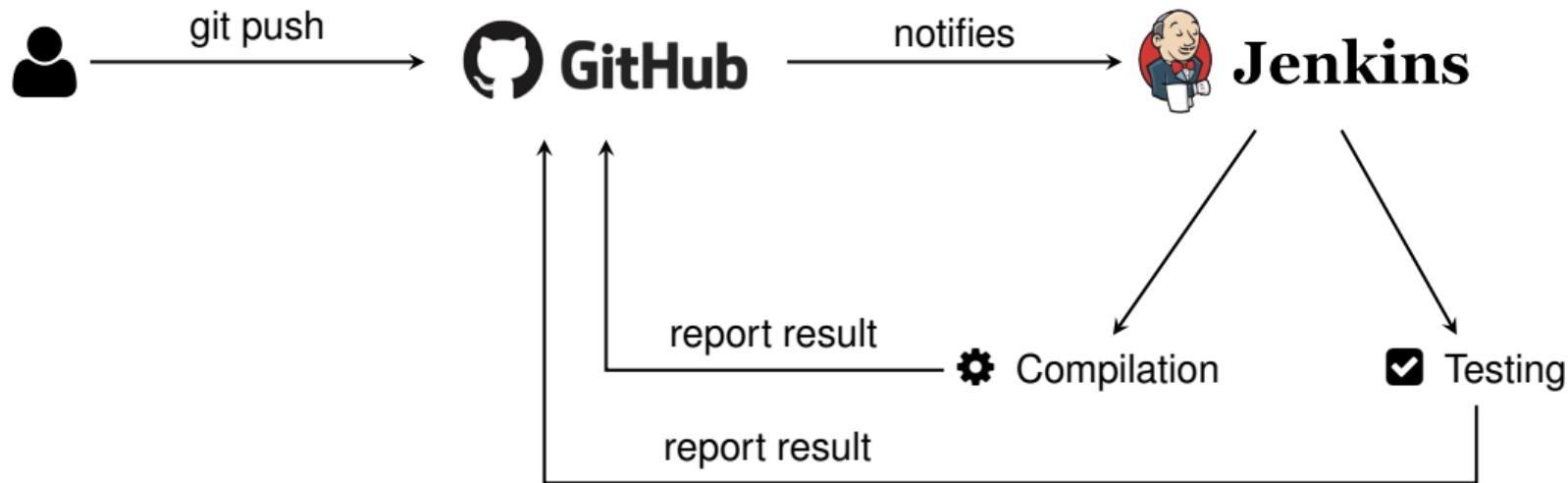
- [1 fixed warning](#)



Static Analysis Warnings: [188 warnings](#).

- [1 fixed warning](#)

# Pull Requests: Automatic Testing



# Pull Requests: Automatic Testing



## All checks have passed

[Hide all checks](#)

4 successful checks



 **lammps/pull-requests/build-docs-pr** — head run ended

[Details](#)



 **lammps/pull-requests/openmpi-pr** — head run ended

[Details](#)



 **lammps/pull-requests/serial-pr** — head run ended

[Details](#)



 **lammps/pull-requests/shlib-pr** — head run ended

[Details](#)



## This branch has no conflicts with the base branch

Merging can be performed automatically.

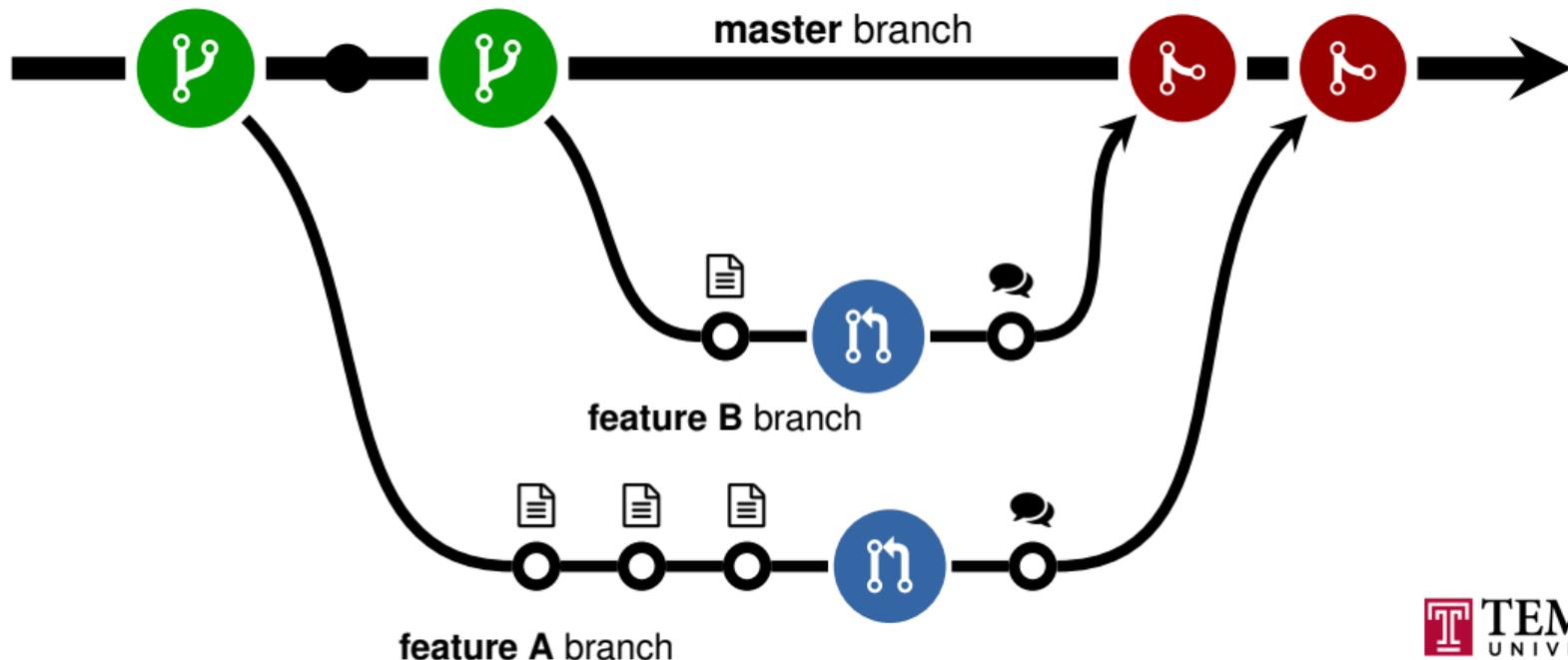
**Merge pull request**



or view [command line instructions](#).

## GitHub Workflow - Multiple Feature Branches

Branches can have different starting points. As long as they have a common point in time, git will try to figure out how to merge these two sequences.



## Feature branches

- ▶ branches allow you to work on more than one topic/feature
- ▶ changes in feature A unrelated to changes in feature B  $\Rightarrow$  use separate branches
- ▶ the time it takes to finish one topic/feature may differ from another
- ▶ by separating them you can more easily merge completed work, without having to complete all the other features you are working on
- ▶ use short descriptive names for branches (e.g. doc\_corrections, fix\_segmentation\_fault, add\_pair\_style\_lj)
- ▶ remember, you can write a more detailed description in the Pull Request

## Real World Examples: AIREBO bugfix

<https://github.com/lammps/lammps/issues/59>

- ▶ Discussions on LAMMPS Mailinglist / Emails to Steve/Axel
- ▶ Multiple independent groups were having issues, some comparing with their own code
- ▶ Issue created on May 12, 2016
- ▶ We fixed some smaller bugs, but we knew it wasn't the root cause
- ▶ A small group of GitHub users assembled, sharing thoughts, code and examples for testing
- ▶ Pull requests followed in the course of the issue discussions
- ▶ One month ago we could finally close this issue



## Commit History in the old workflow

| Release Tag | Date | Commits    | Authors   |
|-------------|------|------------|---|
| r15407      | 305  | 2016-07-30 | <b>sjplimp (289)</b> , athomps (11), stamoor (5)              |
| r15061      | 369  | 2016-05-17 | <b>sjplimp (329)</b> , stamoor (26), athomps (14)             |
| r14624      | 261  | 2016-02-15 | <b>sjplimp (222)</b> , stamoor (24), athomps (15)             |
| r14304      | 368  | 2015-12-08 | <b>sjplimp (286)</b> , athomps (71), stamoor (11)             |
| r13864      | 282  | 2015-08-10 | <b>sjplimp (245)</b> , athomps (25), stamoor (12)             |
| r13475      | 319  | 2015-05-15 | <b>sjplimp (290)</b> , athomps (14), pscrozi (8), stamoor (7) |

- ▶ Attributions would go into README files and [lammeps.sandia.gov/authors.html](http://lammeps.sandia.gov/authors.html)
- ▶ Contributions and Integration work not visible

## Commit History in the new workflow

| Release Tag     | Commits | Authors   |
|-----------------|---------|---|
| patch_24Jul2017 | 144     | Axel Kohlmeyer (74), sjplimp (21), Abdoreza Ershadinia (15), Markus Hoehnerbach (8), Abdo (6), Ryan S. Elliott (5), Giacomo Fiorin (5), Max Veit (4), Steve Plimpton (3), Christoph Junghans (2), H. Metin Aktulga (1)                |
| patch_6Jul2017  | 93      | Axel Kohlmeyer (47), Sebastian Hütter (18), sjplimp (12), Stefan Paquay (6), Steve Plimpton (5), Andrew Jewett (3), Stan Moore (2)  |
| patch_23Jun2017 | 28      | Axel Kohlmeyer (18), sjplimp (5), Steve Plimpton (5)  |
| patch_20Jun2017 | 190     | Axel Kohlmeyer (105), sjplimp (30), Emile Maras (10), Anders Hafreager (10), Lars Pastewka (8), Richard Berger (7), Steve Plimpton (5), Stefan Paquay (5), Stan Moore (4), dstelter92 (3), Oliver Henrich (2), Markus Hoehnerbach (1) |
| patch_19May2017 | 132     | Axel Kohlmeyer (62), DallasTrinkle (22), sjplimp (21), Richard Berger (19), Steve Plimpton (7), Giacomo Fiorin (1)  |
| patch_4May2017  | 39      | Axel Kohlmeyer (25), sjplimp (5), Stan Moore (4), ketankhare (3), Steve Plimpton (2)  |

 Questions?