Software Development on GitHub

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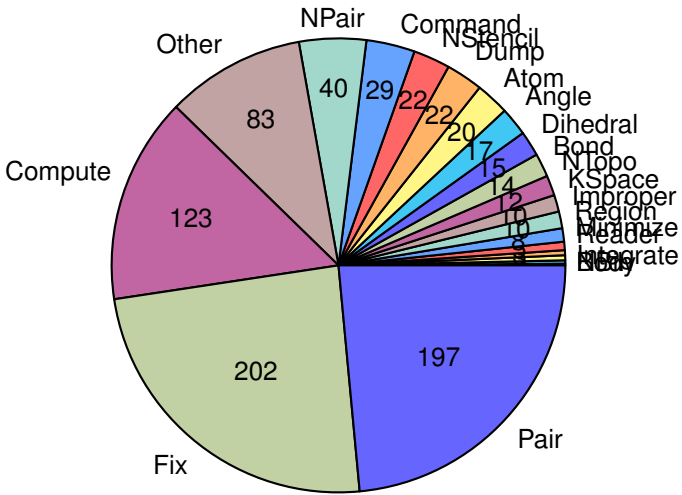
LAMMPS Software Development on GitHub

Target Audience

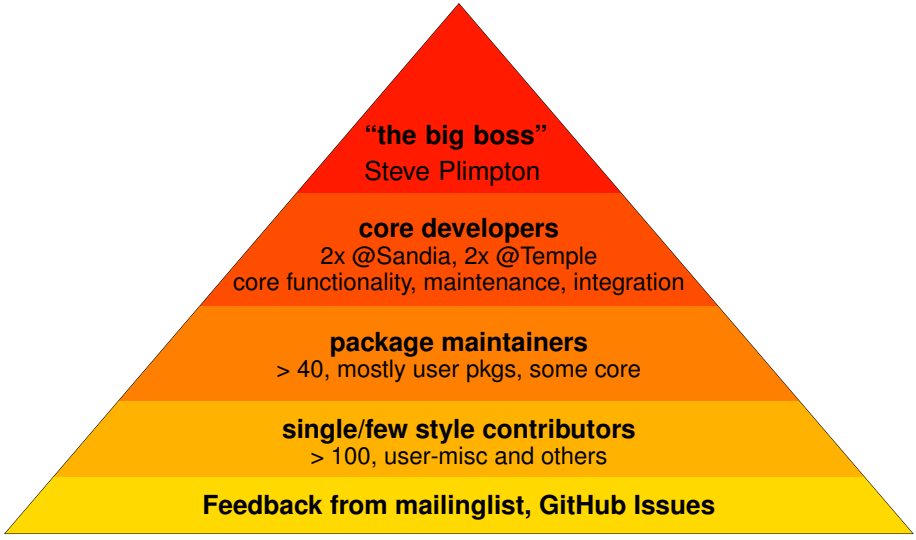
- LAMMPS Developers
- Package Maintainers
- Contributors

LAMMPS in numbers



- ≈800 styles (1250+ if you count accelerator variants)
- 35 packages
- 40 USER packages
- 23 external libraries
- One dozen features enabled through compiler flags (e.g. `-DLAMMPS_PNG`, `-DLAMMPS_FFMPEG`)

LAMMPS Development Pyramid



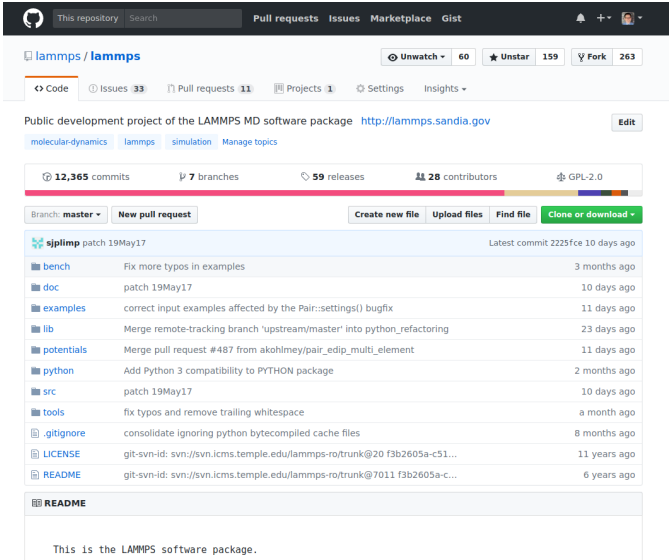
Toolchain

- 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

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

LAMMPS on GitHub



- http://github.com/lammps/lammps
  - public development repository
  - issue tracking
  - contributions are processed as **Pull Requests** for **Code Review** and **Testing**

LAMMPS Development in the **last 3 years**

Since moving to a public development model using GitHub:

- **5600+** commits
- **110+** contributors
- **2.4 million** insertions (+)
- **1 million** deletions (-)

Workflow Documentation

- **LAMMPS Contributing Guidelines**
  https://github.com/lammps/lammps/blob/master/.github/CONTRIBUTING.md

- **LAMMPS GitHub Tutorial**
  http://lammps.sandia.gov/doc/Howto_github.html

Note

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

Release Policy

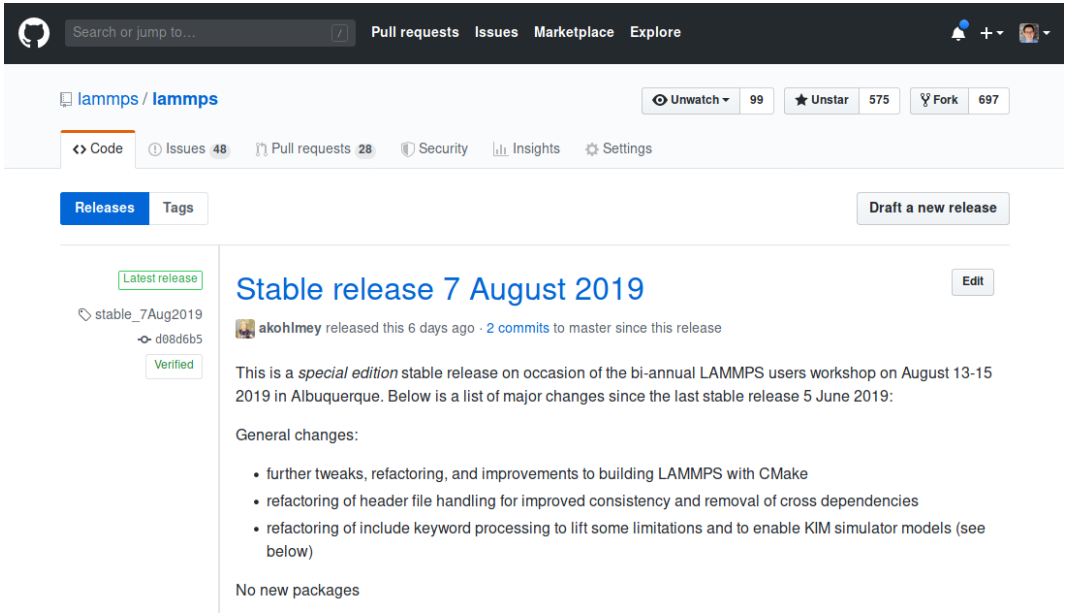
Patch Releases

- a collection of bugfixes and new features
- every few weeks
- posted on website as tarball
- Added as Git tag (e.g. `patch_6Aug2019`)

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
- Added as Git tag (e.g. `stable_7Aug2019`)

Releases on GitHub



Releases on GitHub

In addition there are many small bug fixes, corrections for memory leaks, and memory management inconsistencies, and other general improvements.

Backward compatibility notices:

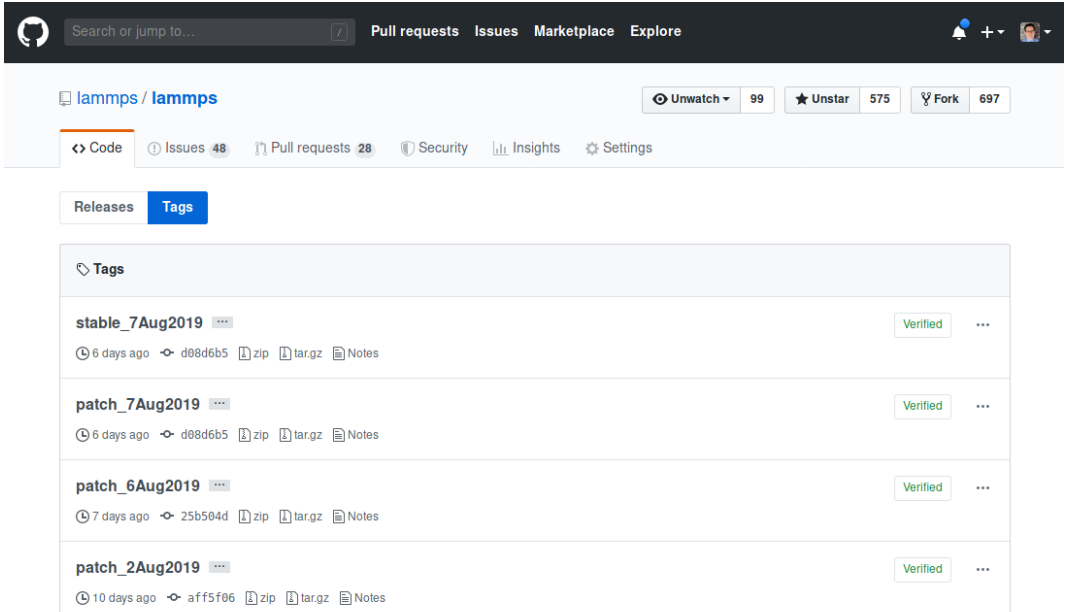
- SNAP parameter files that contain the `diagonalstyle` keyword will generate an error. Solution is to remove the diagonalstyle keyword
- changes in the pair_coeff syntax breaks backward compatibility with inputs using USER-CGDNA. pair style oxdna2/stk has been removed and aliased to oxdna/stk
- restart files using bonded hybrid styles from older LAMMPS versions will not be readable
- the KOKKOS package command keyword gpu/direct was renamed to cuda/aware

Assets 2

Source code (zip)

Source code (tar.gz)

Releases on GitHub



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 to GitHub via Pull Requests

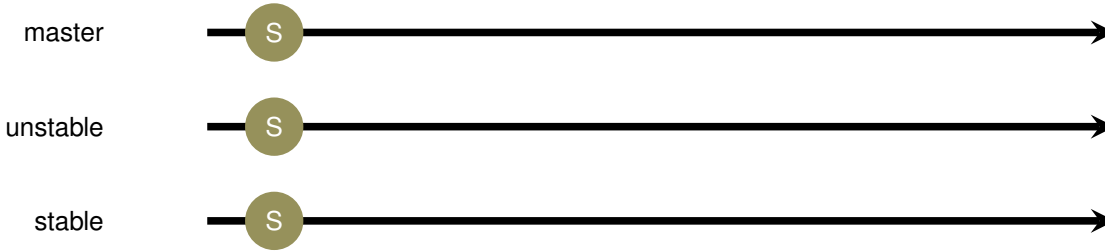
unstable branch

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

stable branch

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

LAMMPS Branches



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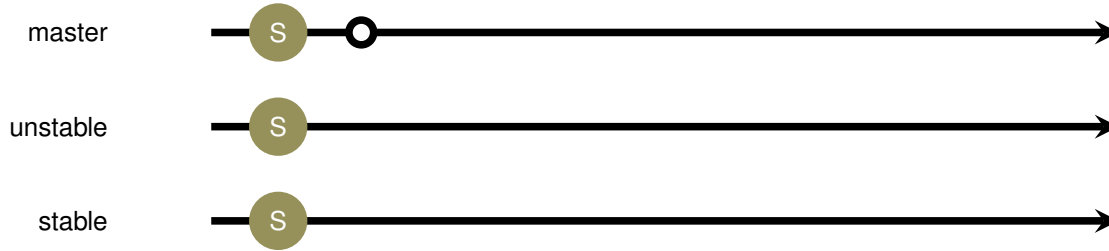

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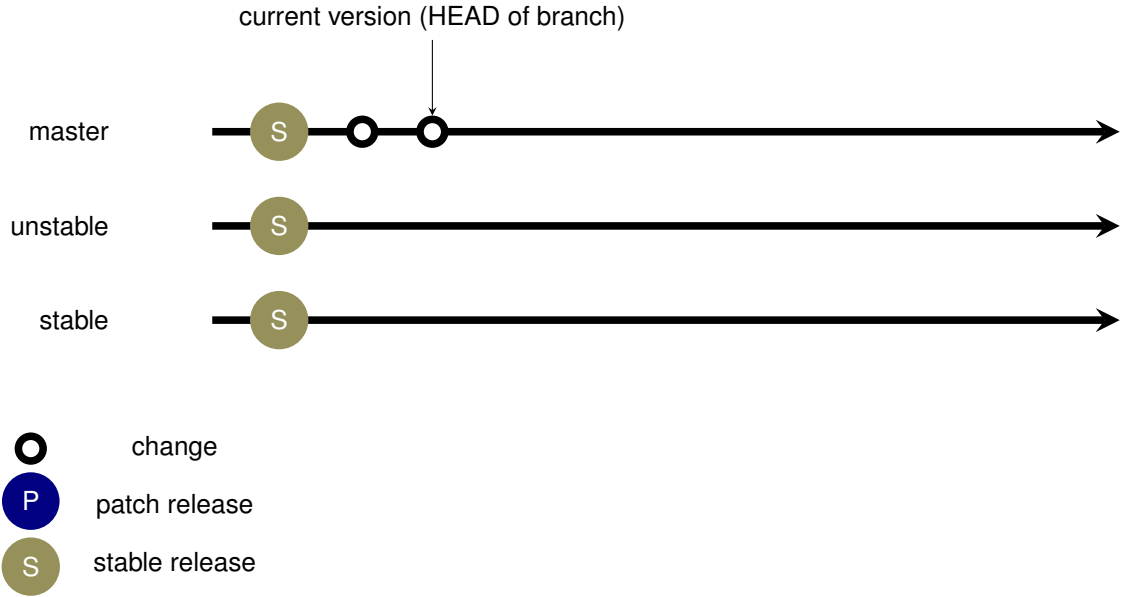

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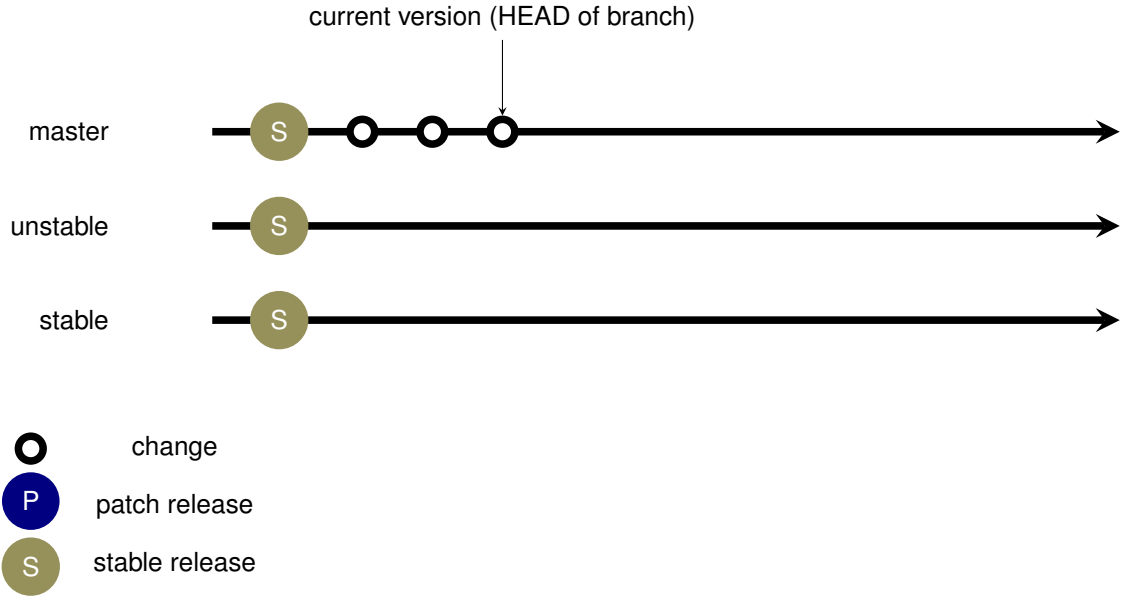

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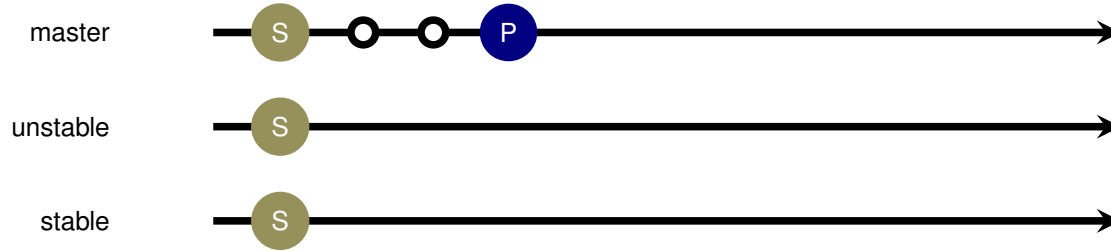

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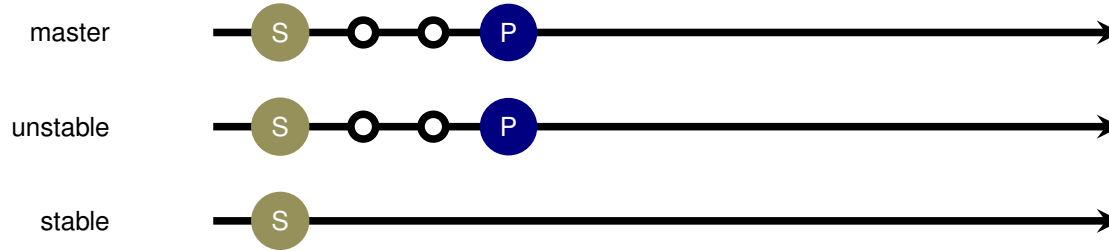

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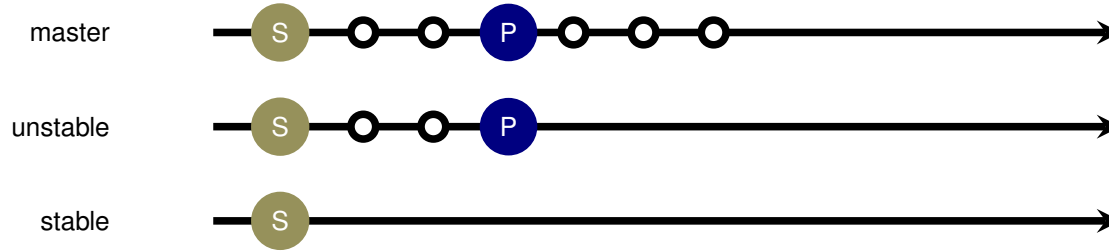

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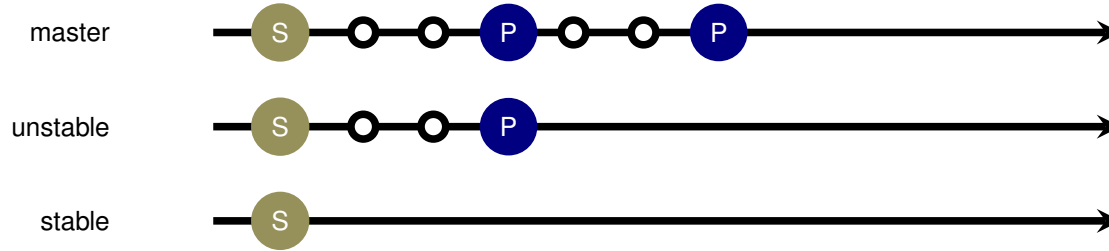

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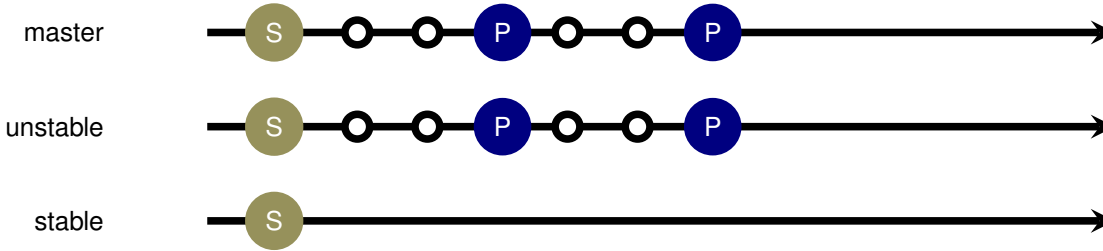

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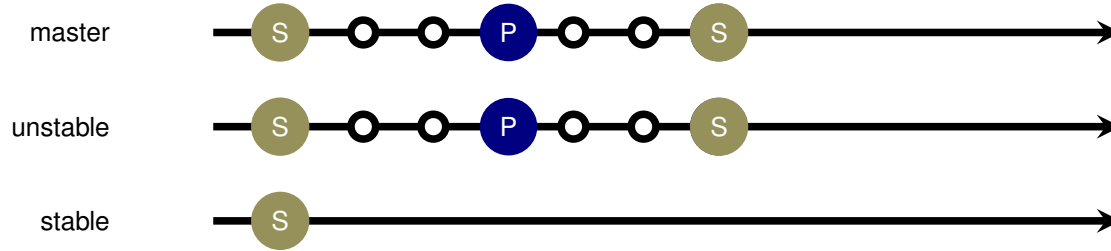

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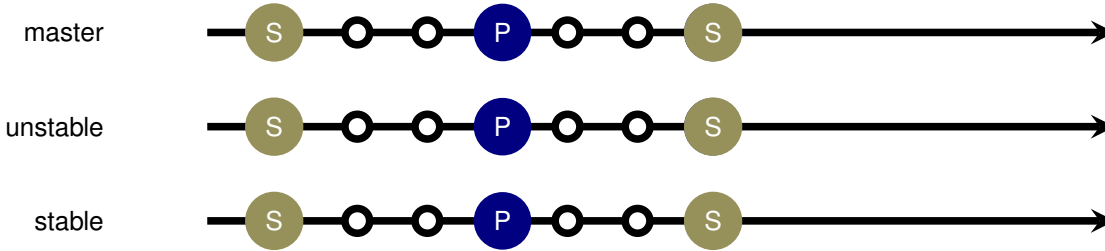

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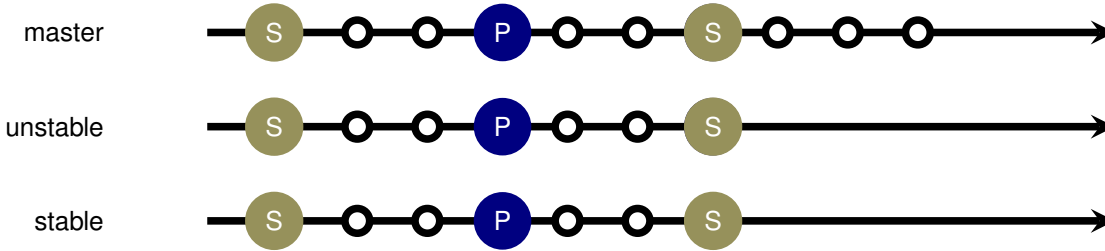

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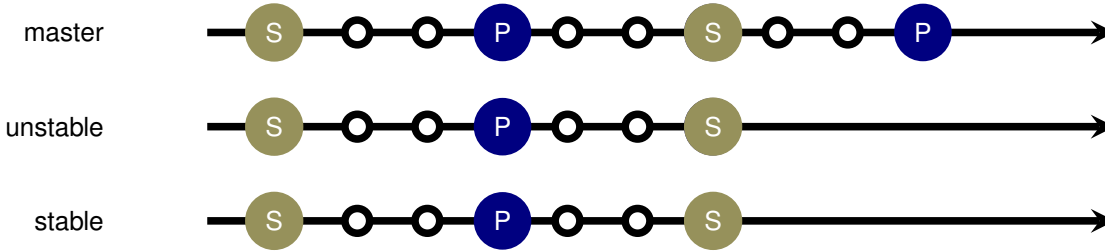

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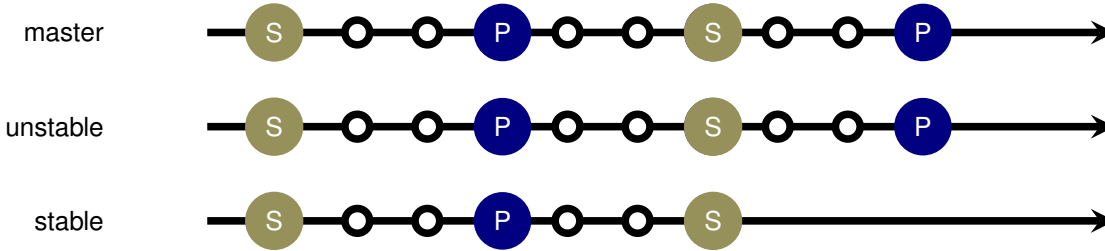

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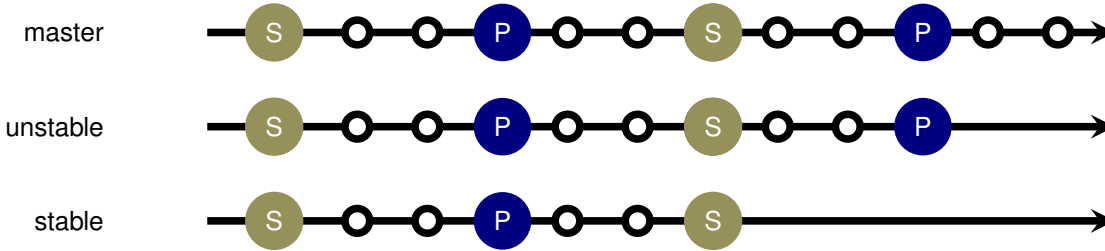


Issue tracking

Usage:

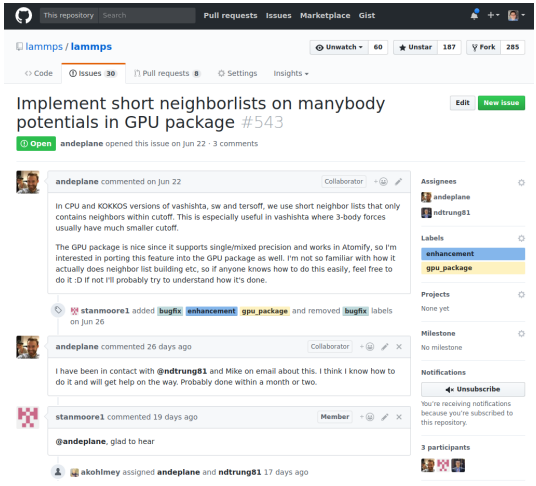
- tracking bugs
- feature requests
- planning new features

Labels

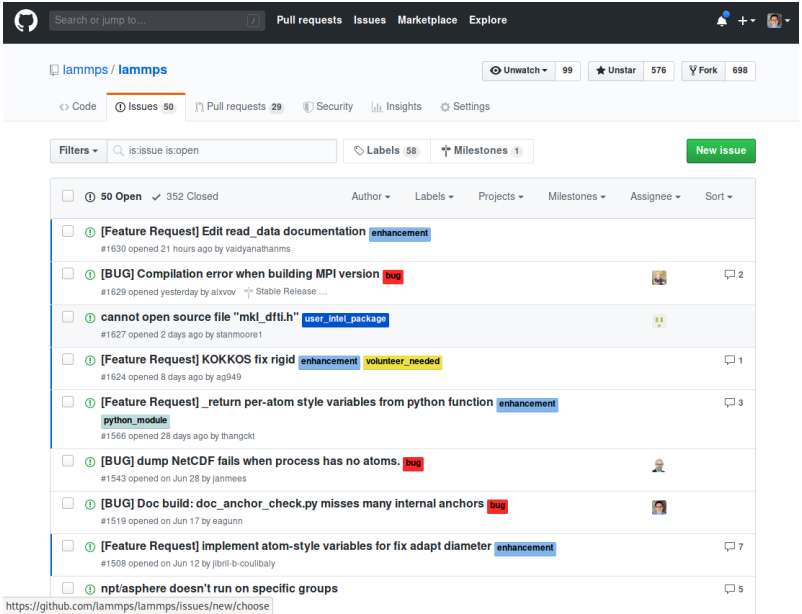
- applied by maintainers
- used to group by topic

Assignment

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



GitHub Issues



GitHub Issue Templates

Bug report
Create a bug report to help us eliminate issues and improve LAMMPS
Get started

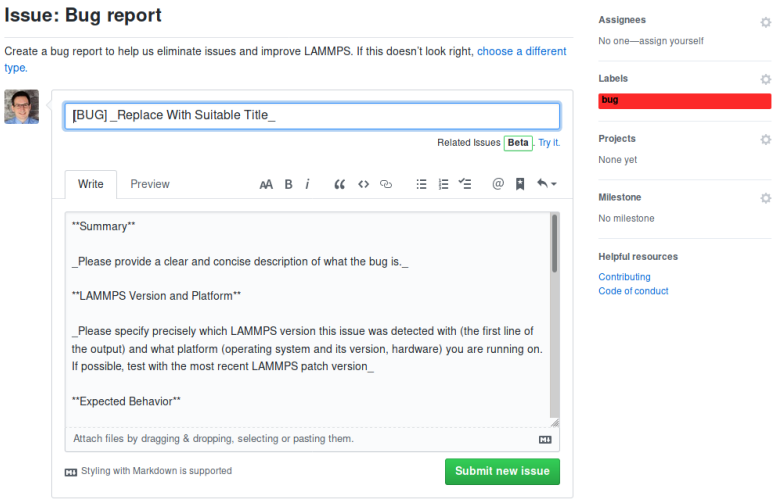
Feature request
Make a suggestion for a new feature or a change to LAMMPS
Get started

Generic Issue
For issues that do not fit any of the other categories
Get started

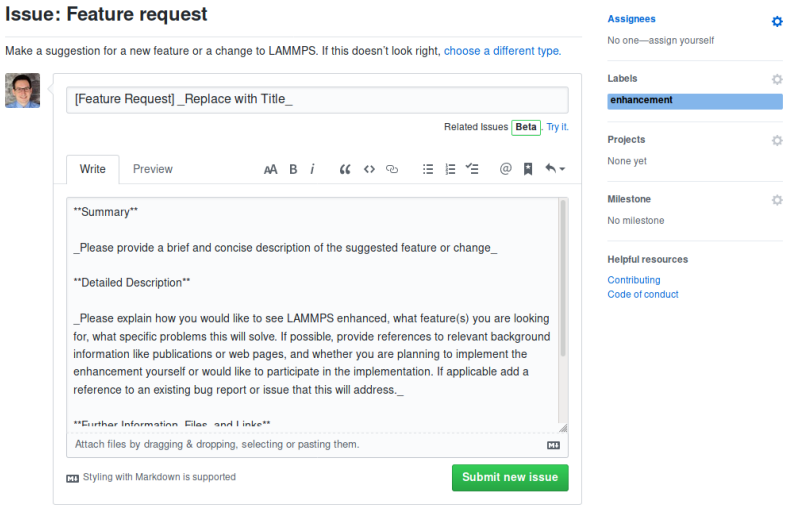
Request for Help
Don't post help requests here, email the lammps-users mailing list
Get started

Don't see your issue here? Open a regular issue.

GitHub Issue Template: Bug Report



GitHub Issue Template: Feature Request



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

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. $\Rightarrow$ 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

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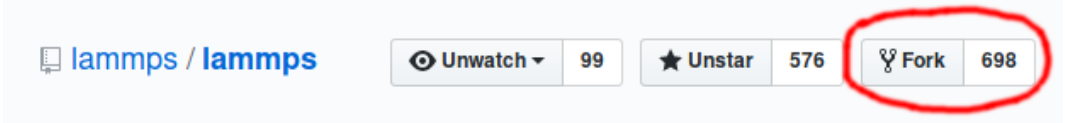
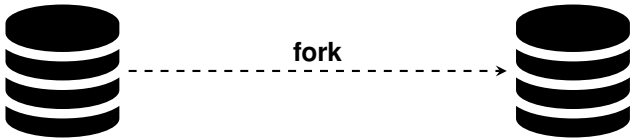
- Or you are implementing a new feature
- What now?

GitHub Workflow

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

GitHub Forks





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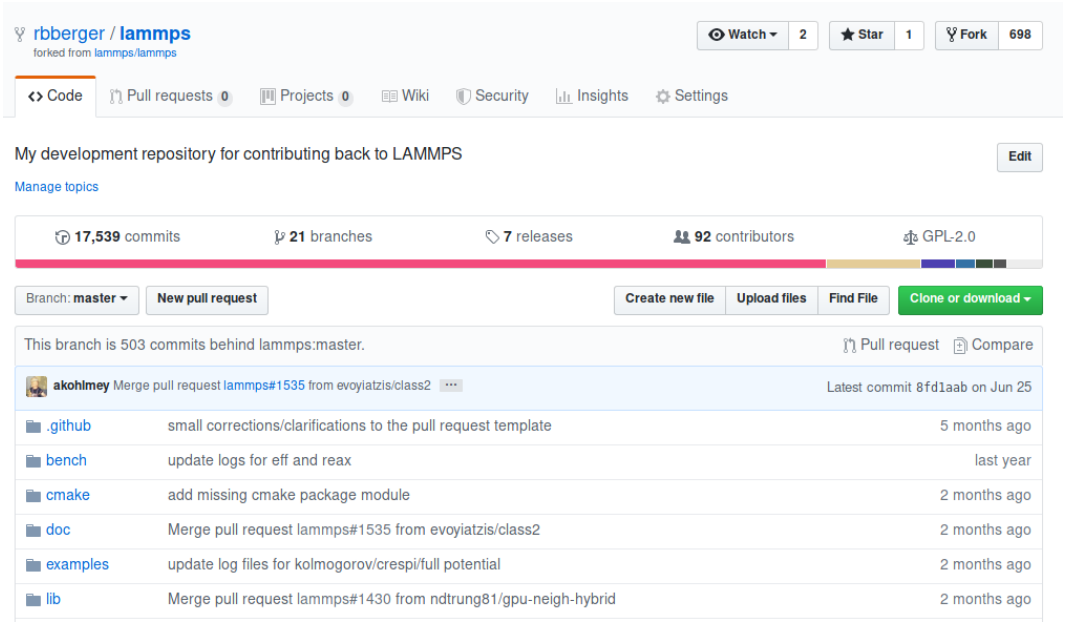

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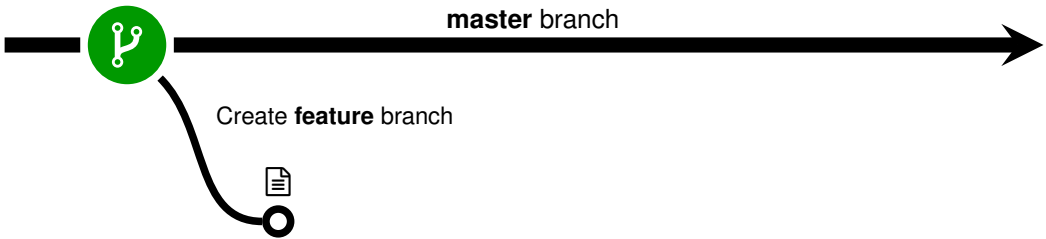

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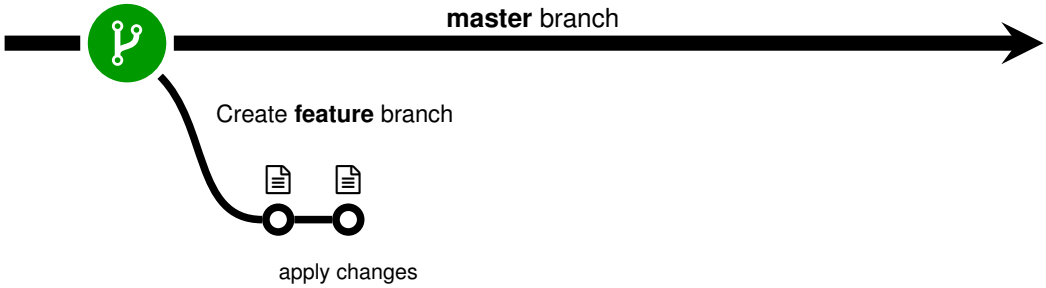

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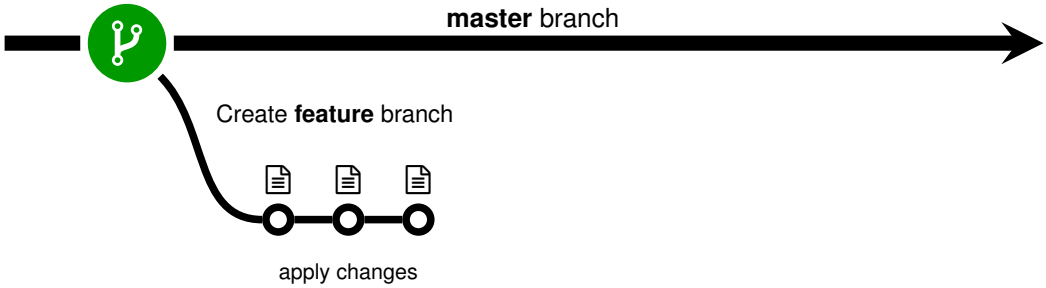

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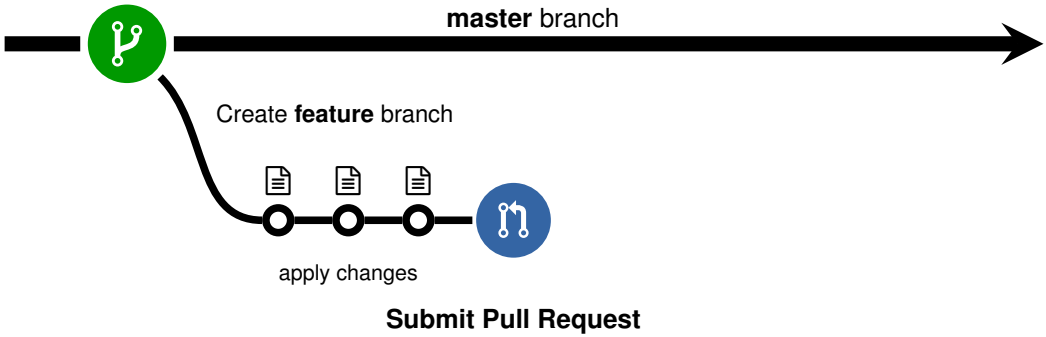

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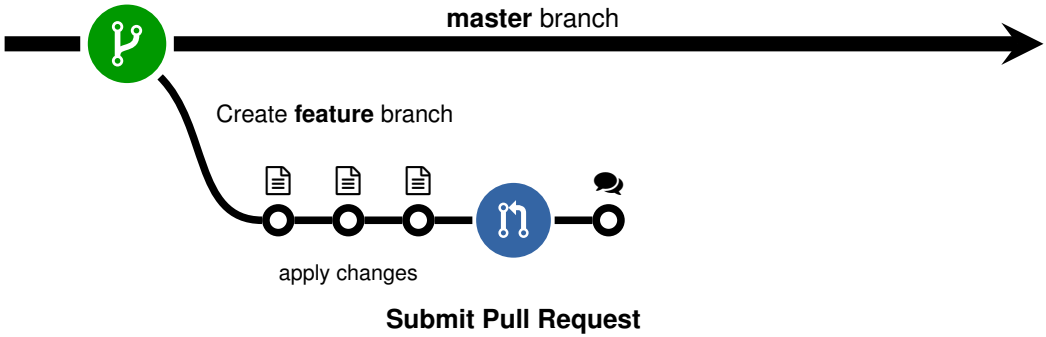

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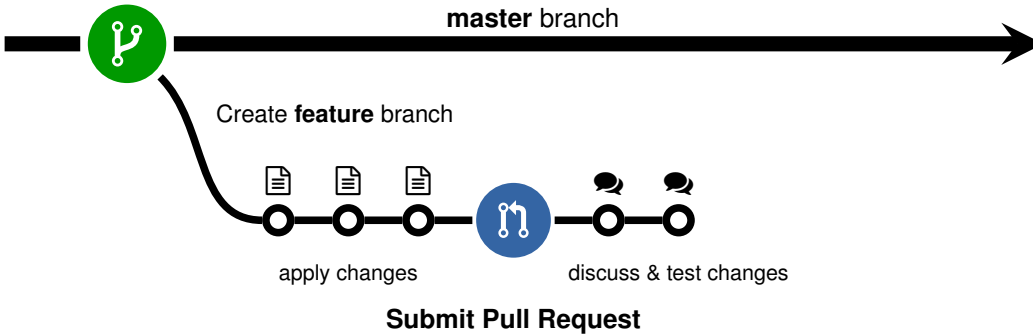

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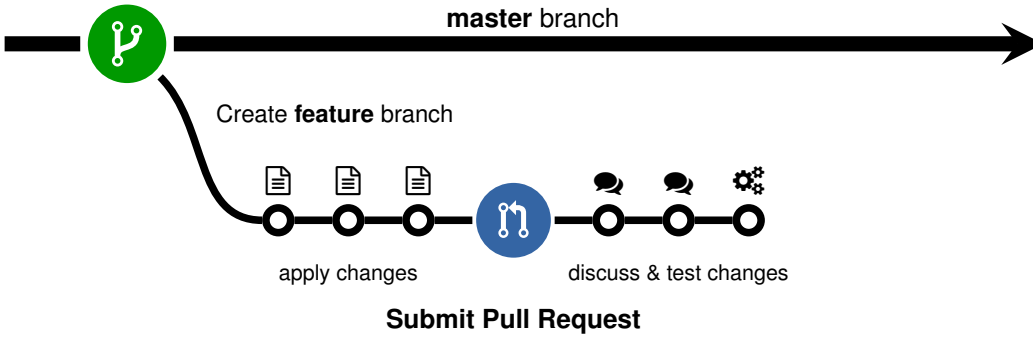

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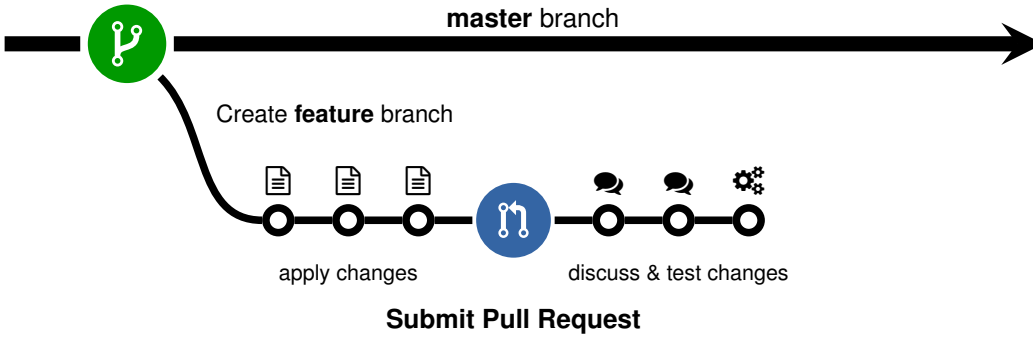

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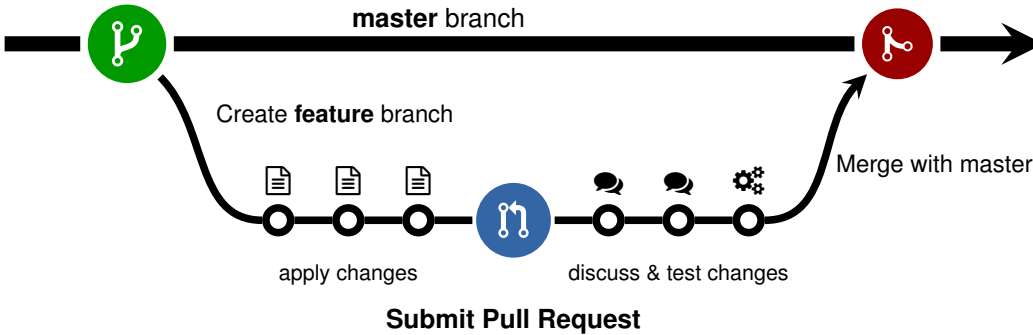
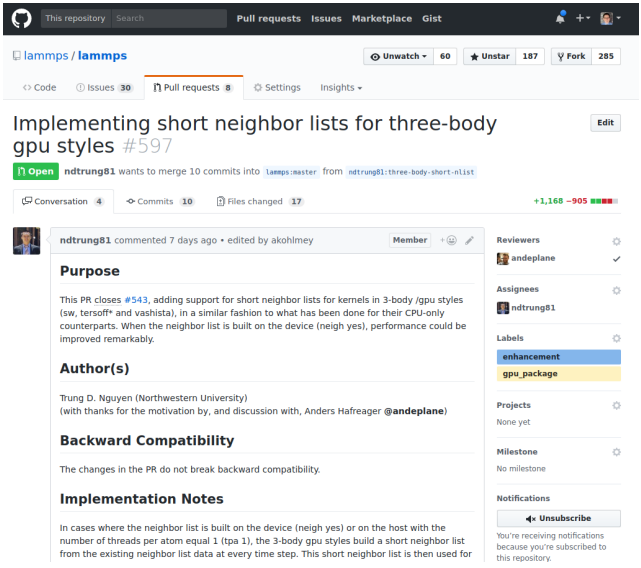
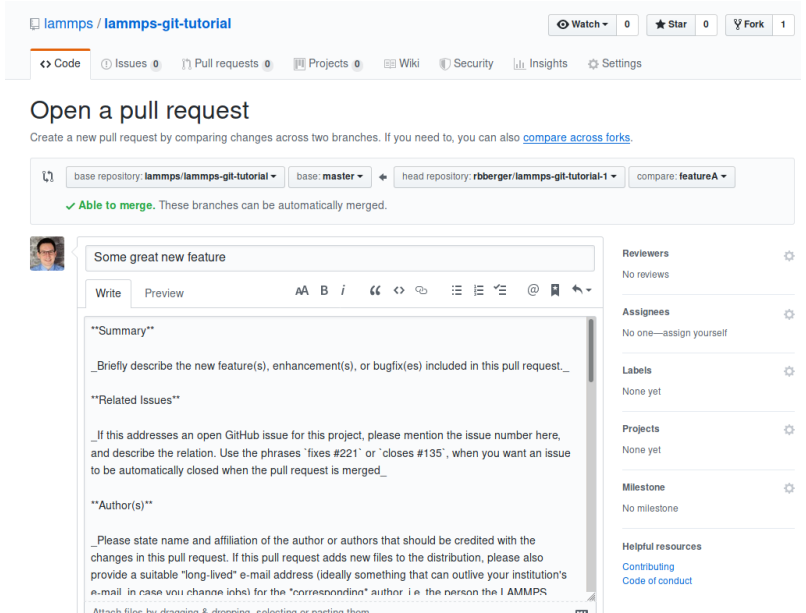


Pull Requests: Contents

- 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

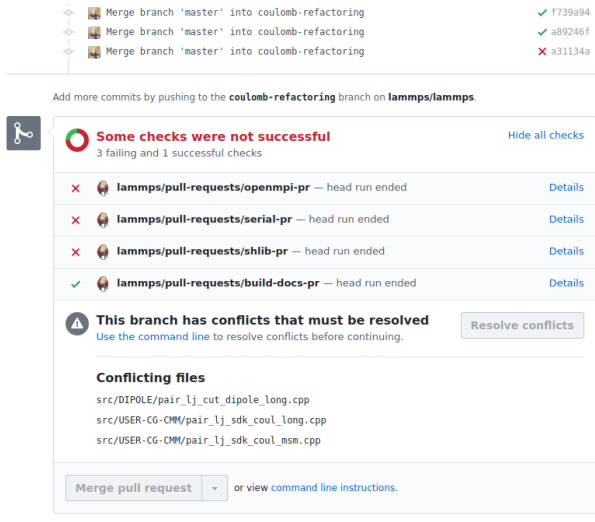


GitHub Pull Request

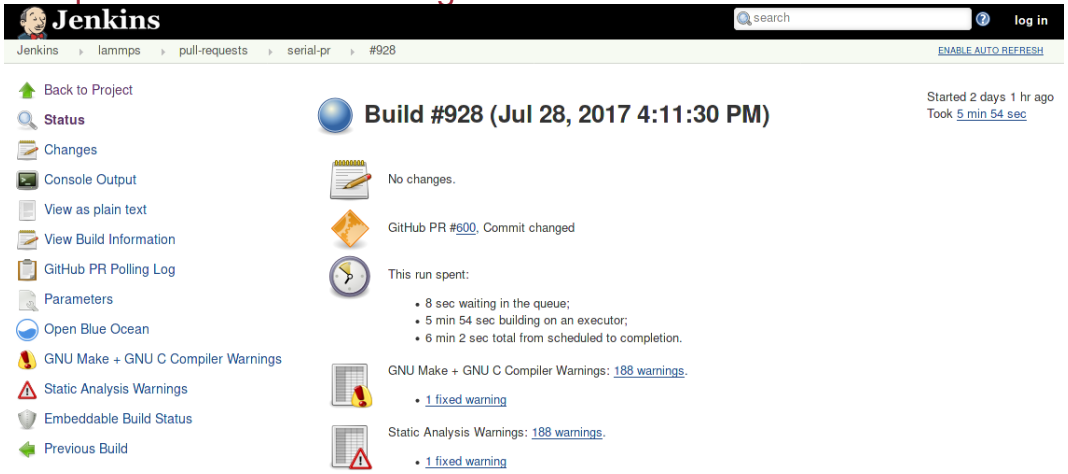


Pull Requests: Automatic Testing

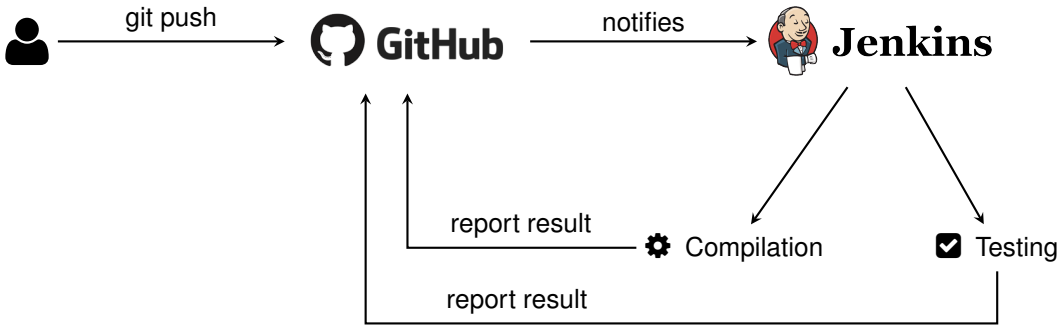
- Once a PR is submitted, your changes will be automatically tested
- Pushing further changes to your branch will be appended to the PR and be tested again
- Click “Details” to get to Jenkins



Pull Requests: Automatic Testing - Jenkins



Pull Requests: Automatic Testing



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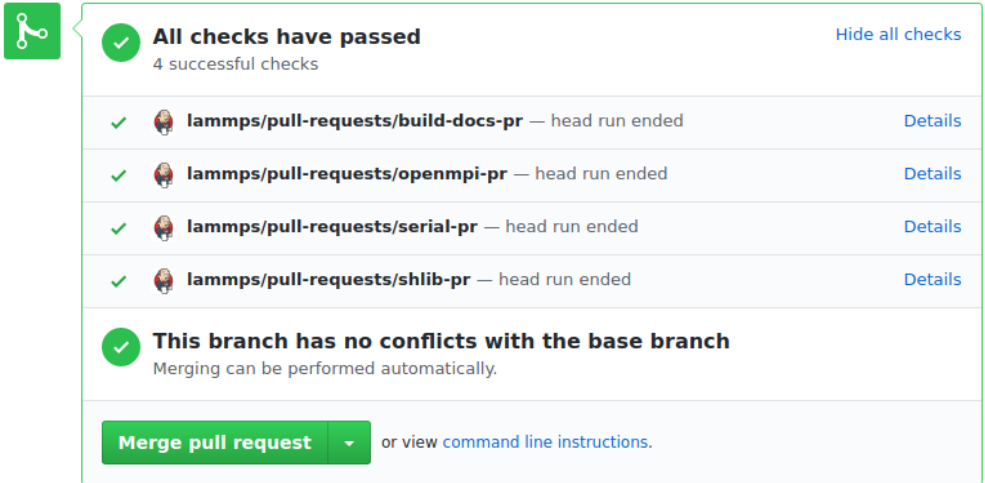


What do we test for?

Containers

- Ubuntu 18.04 LTS
- CentOS 7

Build Systems

- Traditional Make
- CMake + Make

Compilers

- GCC
- Clang
- Intel Compiler

Configurations

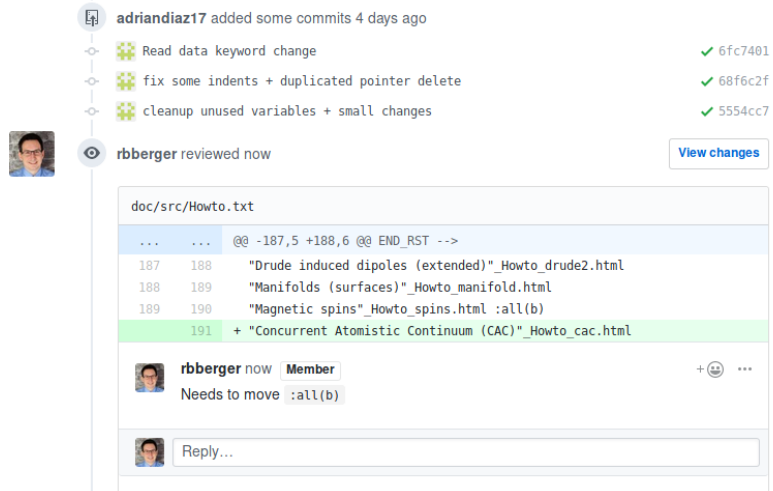
- serial
- MPI
- OpenMP
- GPU
- Other Package combinations

Other

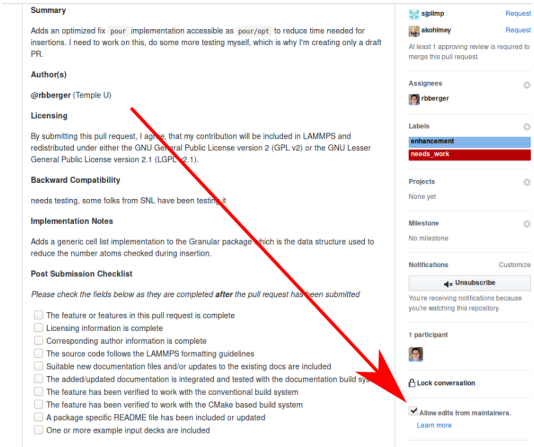
- Documentation / Spell Check
- Static Code Analysis

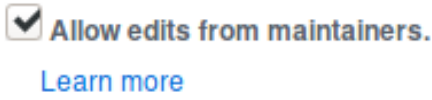
GitHub Code Review

- each part of the code is assigned one or more **Code Owners**
- if your PR touches their code, these people are notified to review your contribution
- they can either **approve**, **comment** or **ask for changes**



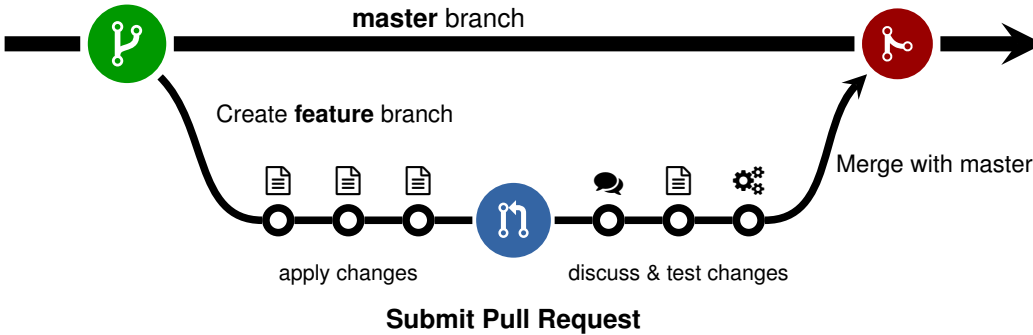
GitHub Pull Requests: Allowing changes by maintainers





- maintainers can push commits to your branch
- simplifies common fixes

GitHub Workflow

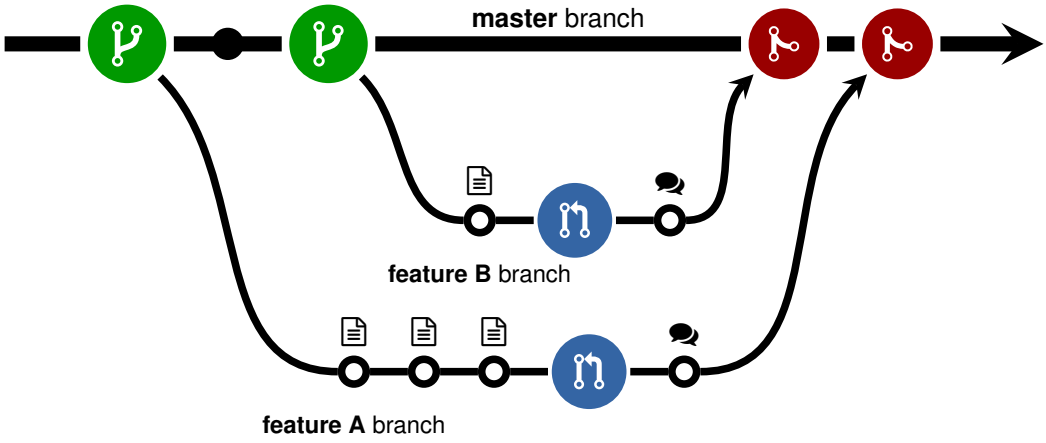


Feature branches

- 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 seperating 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:
  - `doc_corrections`
  - `fix_segmentation_fault`
  - `add_pair_style_lj`
  - ...
- remember, you can write a more detailed description in the Pull Request

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.



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
- After several months we could finally close this issue

Real World Examples: MEAM C++ implementation

https://github.com/lammps/lammps/issues/174

- Issue created on Sep 9, 2016
- A low priority TODO item
- Months later, someone picked it up because they needed it in a new pair style
- A few weeks later we had a complete rewrite

Real World Examples: CMake support

https://github.com/lammps/lammps/pull/573 and many more
https://github.com/lammps/lammps/issues/616 and many more

- Pull Request created on Jul 12, 2017
- Started a discussion between multiple core developers
- I had my own CMake build setup in CMake since 2015, but I alone didn't have the man power to complete the task
- After initial skepticm to get this through Axel and Steve, Junghans and I joined forces
- created a checklist and worked through the issues
- after this initial PR many more followed to gradually improve the build system and its documentation
- Today: "CMake is sometimes a better option for Desktop systems"

Commit History before GitHub

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

- Attributions would go into README files and lammps.sandia.gov/authors.html
- Contributions and Integration work not visible

Commit History (2017)

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)

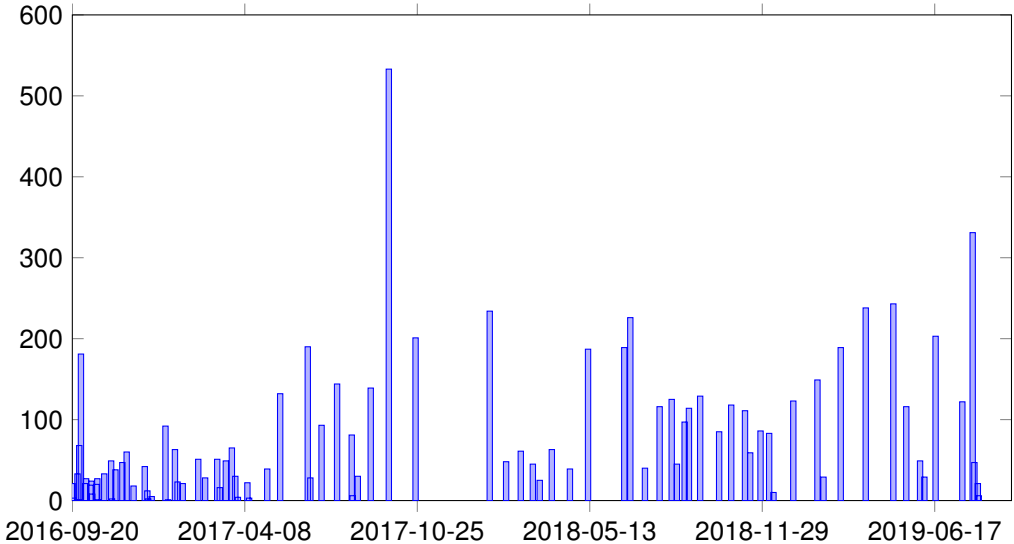
Commit History (2019)

Release Tag	Commits	Authors
stable_7Aug2019	6	Axel Kohlmeyer (5), Steve Plimpton (1)
patch_6Aug2019	21	Axel Kohlmeyer (14), Richard Berger (4), Giacomo Fiorin (2), Ryan S. Elliott (1)
patch_2Aug2019	47	Axel Kohlmeyer (37), Wengen Ouyang (3), Michael Brown (2), Richard Berger (2), Anne Gunn (1), Evangelos Voyiatzis (1), Giacomo Fiorin (1)
patch_31Jul2019	331	Axel Kohlmeyer (204), Ellad Tadmor (37), Ryan S. Elliott (32), Stan Moore (14), Jacob Gissinger (8), Julien Devemy (8), Rupert Nash (8), Evangelos Voyiatzis (6), Steve Plimpton (5), Anne Gunn (2), Denis Taniguchi (2), Ellad B. Tadmor (2), Michal Kanski (2), Adrian Diaz (1)
patch_19Jul2019	122	Axel Kohlmeyer (71), Stan Moore (20), Oliver Henrich (6), Aidan Thompson (5), Sebastian Hütter (4), Evangelos Voyiatzis (3), Anne Gunn (2), Dan S. Bolintineanu (2), Julien Tranchida (2), Trung Nguyen (2), Vishnu V. Krishnan (2), Christoph Junghans (1), Richard Berger (1), Steve Plimpton (1)
patch_18Jun2019	203	Stan Moore (61), Axel Kohlmeyer (57), Julien Tranchida (32), Aidan Thompson (21), Richard Berger (13), Vishnu V. Krishnan (4), Evangelos Voyiatzis (3), Trung Nguyen (3), Gareth Tribello (2), Jacob Gissinger (2), Adrian Diaz (1), Christoph Junghans

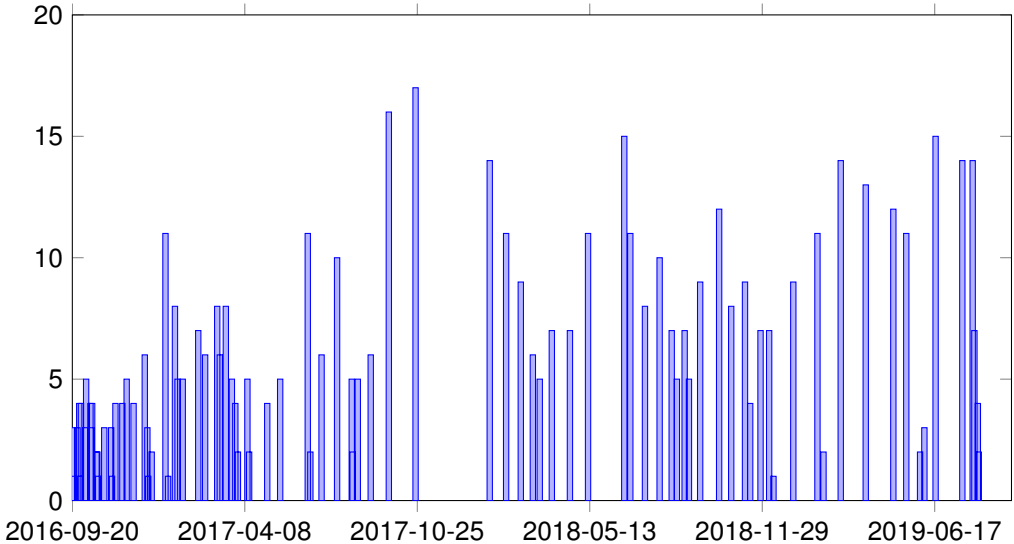
Recent Commit History

Release Tag	Commits	Authors
stable_7Aug2019	730	Axel Kohlmeyer (388), Stan Moore (95), Ellad Tadmor (37), Julien Tranchida (34), Ryan S. Elliott (33), Aidan Thompson (26), Richard Berger (20), Evangelos Voyiatzis (13), Jacob Gissinger (10), Julien Devemy (8), Rupert Nash (8), Steve Plimpton (7), Oliver Henrich (6), Vishnu V. Krishnan (6), Anne Gunn (5), Trung Nguyen (5), Sebastian Hütter (4), Giacomo Fiorin (3), Michal Kanski (3), Wengen Ouyang (3), Adrian Diaz (2), Christoph Junghans (2), Dan S. Bolintineanu (2), Denis Taniguchi (2), Ellad B. Tadmor (2), Gareth Tribello (2), Michael Brown (2), Kamesh AK (1), Sam Niblett (1)
stable_5Jun2019	1165	Axel Kohlmeyer (718), Ryan S. Elliott (68), Julien Tranchida (50), Dan S. Bolintineanu (45), Steve Plimpton (41), Jacob Gissinger (33), Stan Moore (24), Mingjian Wen (22), Evangelos Voyiatzis (20), Michal Kanski (18), Steven Strong (14), Sebastian Hütter (13), Norbert Podhorszki (11), Risto Toijala (10), Jan Janßen (8), Agilio Padua (6), Richard Berger (6), Aidan Thompson (5), Christoph Junghans (5), Steven Vandenbrande (5), casievers (5), pmla (5), Wengen Ouyang (4), Adrian Diaz (3), Giacomo Fiorin (3), Oliver Henrich (3), Donatas Surblys (2), Lars Pastewka (2), PabloPiaggi (2), Zbigniew Koziol (2), charlie sievers (2), efetis (2), Cyril Falvo (1), Diaz (1), Eisuke Kawashima (1), Eugen Rožić (1), Michael Brown (1), Theophile Chirac (1), Vishal Boddu (1), ckadding (1)
stable_12Dec2018	892	Axel Kohlmeyer (431), Steve Plimpton (102), Stan Moore (81), Rene Halver (49), Richard Berger (42), Christoph Junghans (30), Jacob Gissinger (28), Gareth Tribello (26), Denis Taniguchi (15), Stefan Paquay (12), Sergey Lishchuk (11), Daniel Schwen (10), ckadding (10), Aidan Thompson (8), Michele Invernizzi (6), dilkins (4), pmla (4), Michael Brown (3), Giacomo Fiorin (2), Michal Kanski (2), Morteza Jalalvand (2), Oliver Henrich (2), PabloPiaggi (2), RomainVermorel (2), Sebastian Hütter (2), Wengen Ouyang (2), Diego Ugarte (1), Pierre de Buyl (1), araven (1), oywg11 (1)
stable_22Aug2018	1030	Axel Kohlmeyer (338), Steve Plimpton (240), Julien Tranchida (83), Richard Berger (78), Christoph Junghans (71), Jacob Gissinger (43), Trung Nguyen (43), Stan Moore (24), Stefan Paquay (20), PabloPiaggi (12), Charlles Abreu (8), Wengen Ouyang (8), Christian Negre (7), Michael DeLyser (6), Sebastian Hütter (6), David Nicholson (5), Ryan S. Elliott (5), araven (5), HaoZeke (4), Oliver Henrich (3), robeme (3), Julien Devemy (2), MICHAEL ROBERT DELYSER (2), Marshall McDonnell (2), Tim Mattox (2), Tomáš Trnka (2), Aidan Thompson (1), Amrita

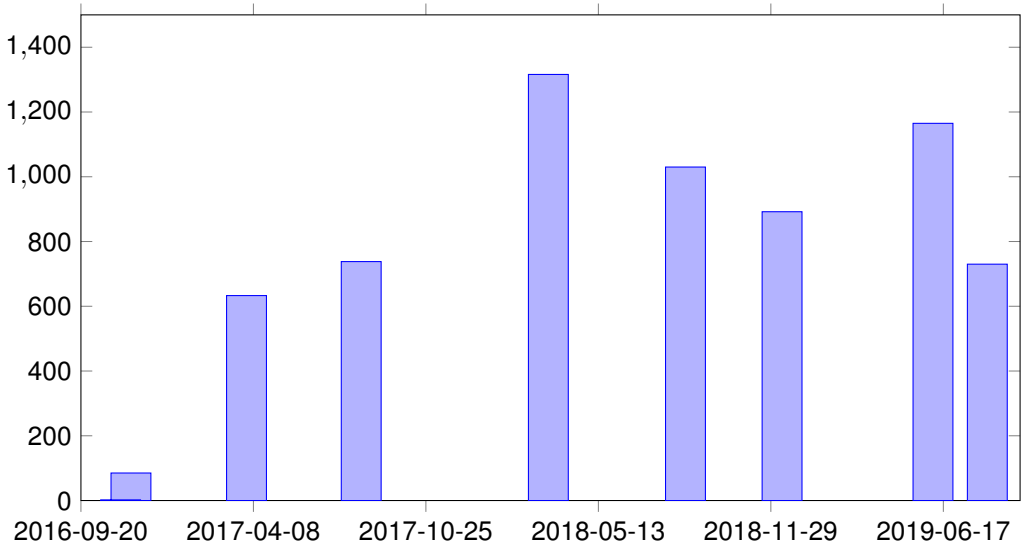
Number of Commits in Releases (Patch+Stable)



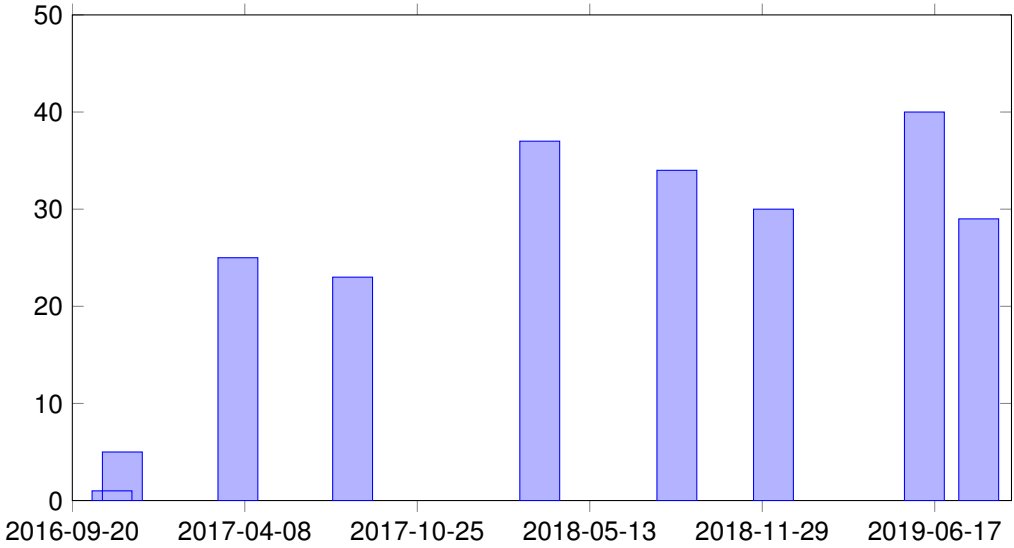
Number of Contributors in Releases (Patch + Stable)



Number of Commits in Stable Releases



Number of Contributors in Stable Releases



Questions?