Helping build a developer community though good software practice

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HPC Carpentry for Chemists, University of Mauritius, August 20, 2021

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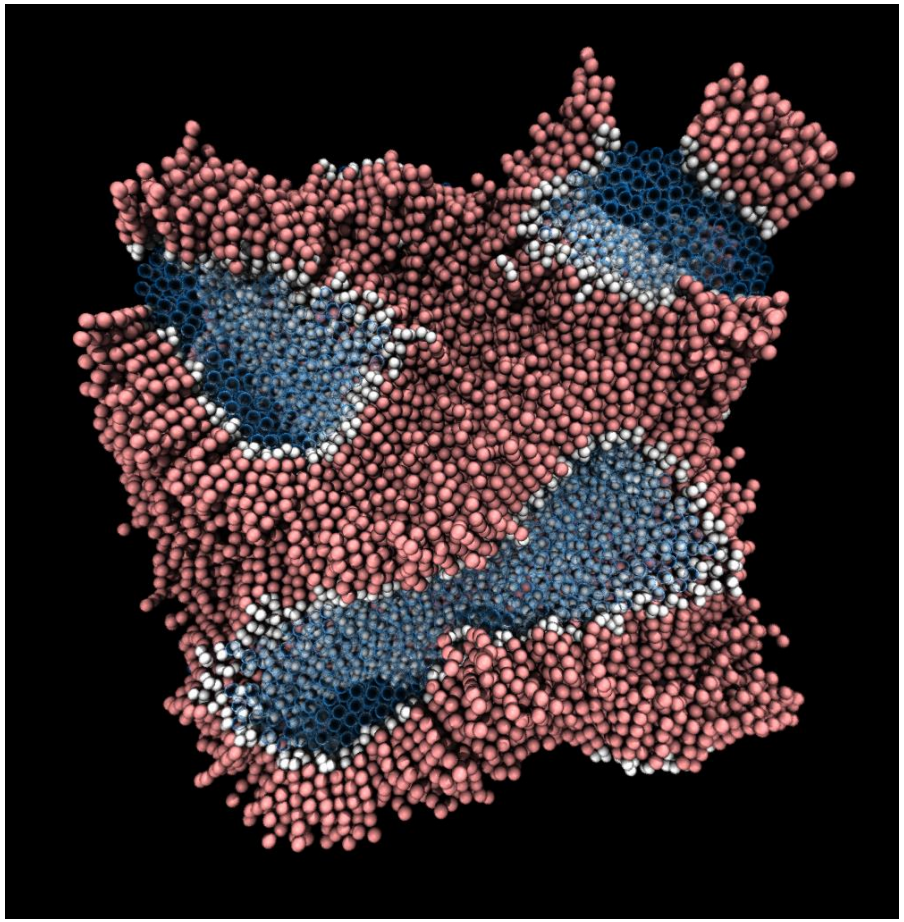
Lessons from GROMACS evolution - biomolecular simulation



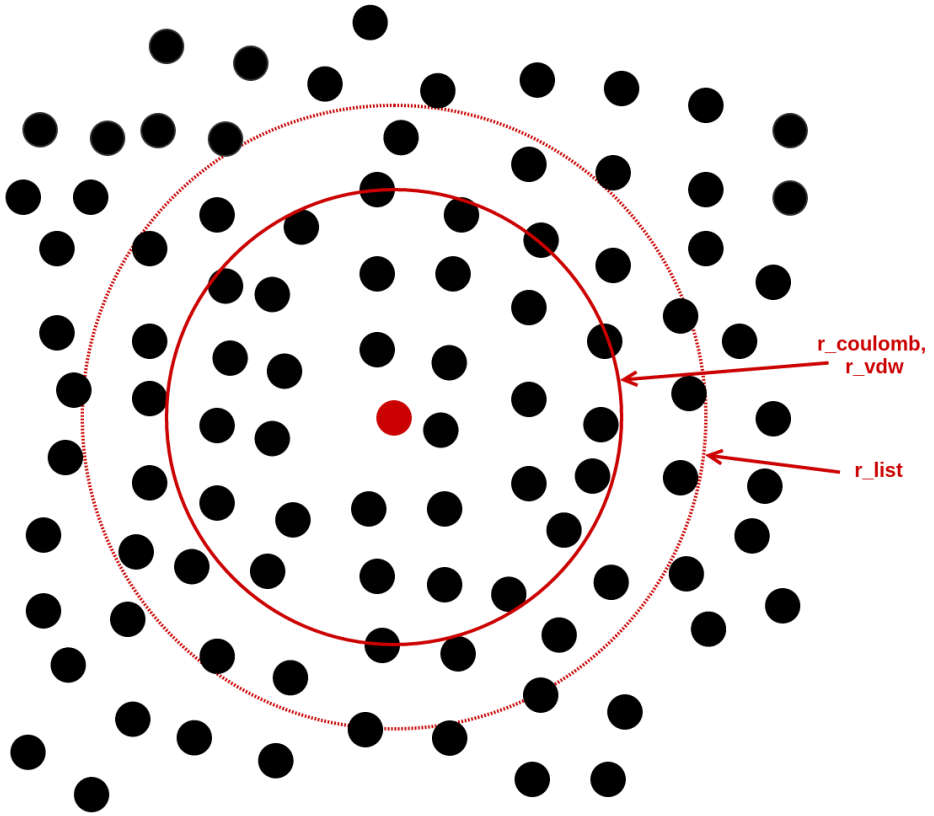
Humble origins

- Originally a **hardware** project at the University of Groningen in the early 1990s – custom-designed 32-processor ring using PVM
- Design and simulation methodology largely adopted from existing GROMOS molecular simulation package
- **Key decision**: write in a language that suits the problem you want to solve and where you want to spend your time

Early software practice

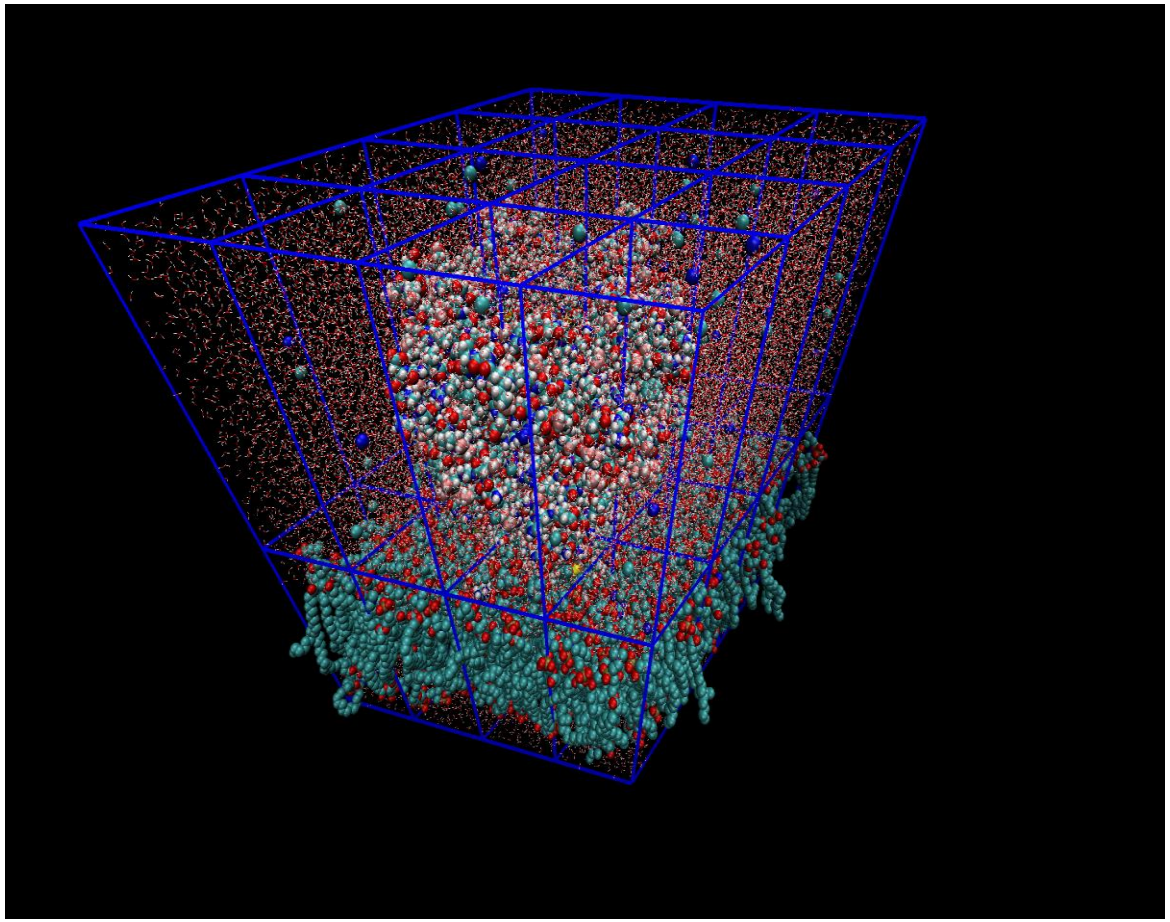
- First public release – 2.0 some time in the 1990s
- First paper – “GROMACS: a message-passing parallel molecular dynamics implementation” *Comp. Phys. Comm.* 1995
- **Key decision**: use version control – first CVS commit in 1997, already 750 files and 145k LOC
- **Key decision**: first FOSS release – 3.0 in August 2001, GPL 2.0
- **Key decision**: provide preparation and analysis tools along with the core simulation engine

N-body neighbor lists



Software practice evolves

- **Key decision**: Use issue tracking, Bugzilla introduced summer of 2005
- **Key decision**: Develop a regression test suite 2007
- **Key decision**: Switch to git for distributed version control (June 2009)
- **Key decision**: Rewrite parallelism layer, keeping the old one working

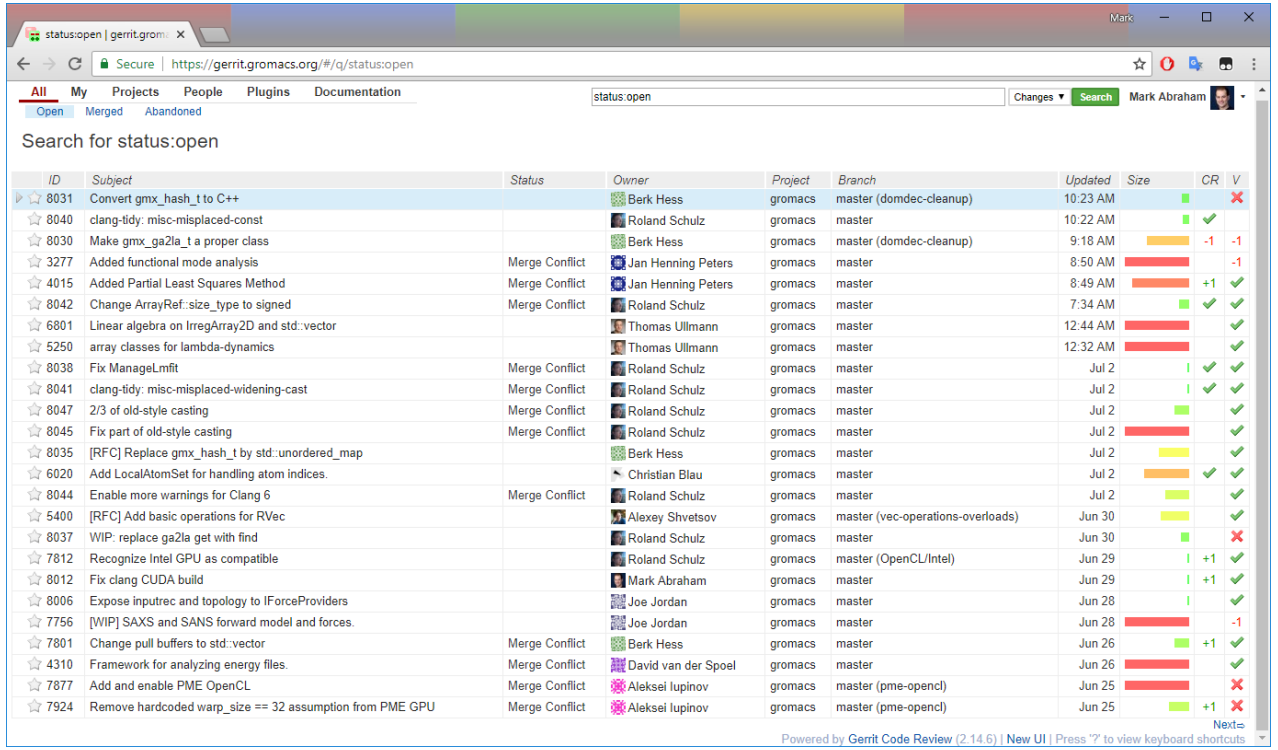


Software practice evolves…

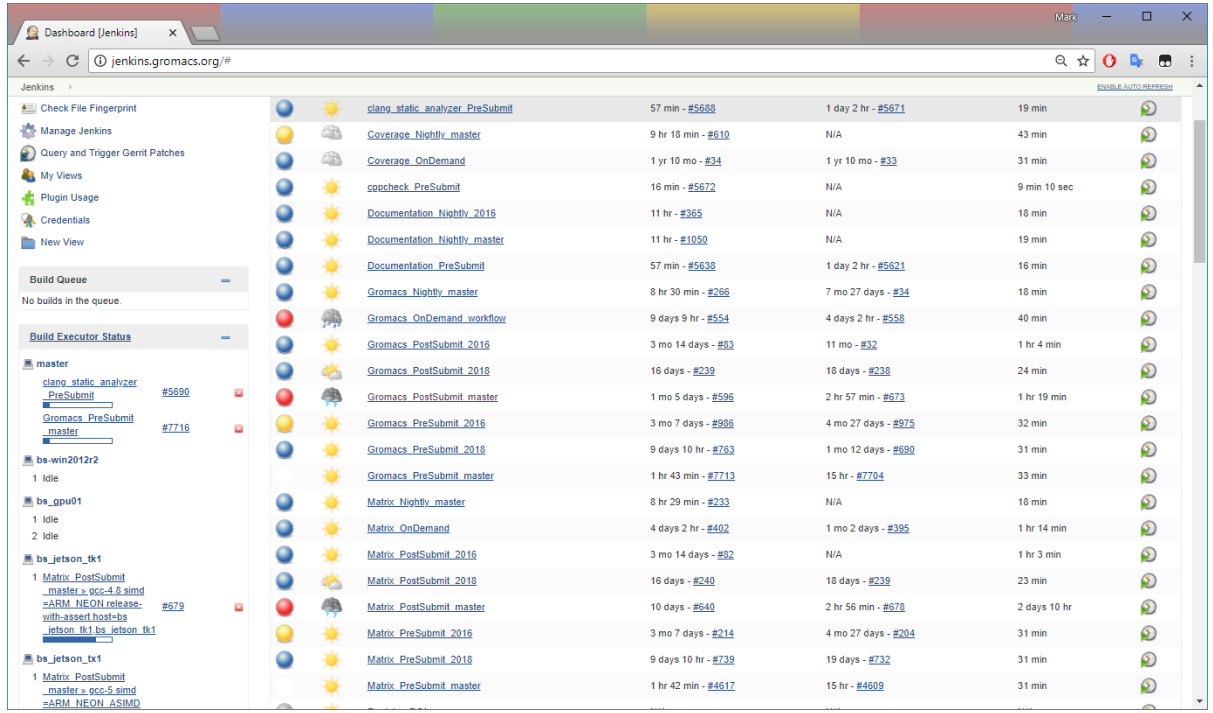
- Because of the high performance, portability, and usability, usage grew
- User community included also many with desire to modify the code and contribute back
- Many new contributors permitted to push to the central git repository over 2008-2010
- Note: not all contributions need to be new code!
- **Key decision**: unite documentation git repository with source code repository (2013)

Growth problems!

- A large community of developers who are not dog-fooding each other's code will break everything, all the time
- Many new code paths led to many bugs, some of them subtle
- **Key decision**: introduce open code review (2011) before changes are accepted – https://gerrit.gromacs.org
- **Key decision**: everybody's changes must be reviewed by others, including changes from the long-term developers (who were mostly now busy professors)



More problems!



- Portability requires ongoing testing
- Developers want to use their laptops, but HPC clusters and distributed computing environments look very different
- **Key decision**: Use continuous-integration testing, which must pass before code is considered for acceptance (2012), including static and dynamic analyzers and linting
- **Key decision**: require unit test for new functionality, add coverage also when modifying old functionality

Recent developments

- **Key decision**: Refactor to support a long-term stable API, callable from C++ and Python, easing pressure for non-core developers to want to contribute to the core, and reducing burden on core developers
- **Key decision**: switch to GitLab so everything is under one roof
- **Key decision**: use containerization to reduce CI maintenance burden

Lessons for your developer community

- Rome wasn't built in a day – pick the battles that suit the current state of your project, the needs of your users, and the resources you can afford
- Automation of processes pays off well
- Pre-commit CI testing makes bug hunting easier – you know you can go back in time, build the old code and it will work
- If you need more performance, consider your algorithms and data structures, match them to the capabilities of the target hardware.
- Plan first how you will test that your code is correct!

Thank you!

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