The evolution of software practice in GROMACS to suit both the laptop and the exascale

PASC 2018, Basel

Mark Abraham, KTH, Sweden

Email: mark@bioexcel.eu
Twitter: @the_mabraham
Biomolecular simulations with GROMACS
GROMACS impact

GROMACS paper citations on Google Scholar per year

- Blue: 2
- Red: 3
- Orange: 3.3
- Green: 4
- Purple: 4.5
- Red: 4.6
- Pink: 5.1
- Green: Total
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**: develop in ANSI C, rather than FORTRAN
- Early adopters and core developers:
  - David van der Spoel, Berk Hess, Anton Feenstra, Rudi van Drunen
Early software practice

- First public release – 2.0 some time in the 1990s
- **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
- **Key decision:** aim for performance portability… x86(!) assembly(!) for key kernels
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 from particle decomposition to domain decomposition
- **Key decision**: Support dynamic load balancing of work between domains
- **Key decision**: Separate long-ranged component of electrostatics to run on dedicated MPI ranks
Dynamically load balanced 3D domain decomposition, GROMACS 4.0
MPMD execution flow
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
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](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).
### Code review... before github

![Image of a code review interface using GitLab](https://bioexcel.eu)

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<th>ID</th>
<th>Subject</th>
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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
- **Key decision**: Include static and dynamic analysis (cppcheck, Sanitizers) and linting (uncrustify)
- **Key decision**: switch to C++ (first C++98, now C++11)
- **Key decision**: require unit test for new functionality, add coverage also when modifying old functionality
Jenkins CI testing
More problems!

• Dennard scaling breakdown leads to multicore and wide-SIMD era
• Impossible to just write serial code and hope for improvement from clock frequency and/or compiler magic
• GPU coding requires this
• **Key decision:** re-cast core algorithms and data structures to match hardware capabilities (2012)
• **Key decision:** use compiler intrinsics for SIMD support, and extract a low-level SIMD layer for each supported platform, in which we implement performance kernels, with full unit test coverage (2014)
4x4 non-bonded neighbor lists
Recent developments

• **Key decision**: Support OpenCL as well as CUDA (2015)
• **Key decision**: Adopt physical validation tests (2017)
• **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 to review, test, and maintain MLOC of others code (work in progress)
• **Key decision**: use containerization to reduce Jenkins maintenance burden, while permitting coverage increase
Lessons for your software team

• 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 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!
Acknowledgments

Far too many to mention, and many didn’t touch the code!

Paul Bauer
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