DUNE as an Example of Sustainable Open Source Scientific Software Development

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In this paper we describe how DUNE, an open source scientific software framework, is developed. Having a sustainable software framework for the solution of partial differential equations is the main driver of DUNE’s development. We take a look how DUNE strives to stay sustainable software.

1 The Cause for DUNE’s Development

DUNE, the “Distributed and Unified Numerics Environment” [5, 2, 1, 3] is a modular software toolbox for solving partial differential equations. When initiating DUNE the rule in scientific software development was that PhD students were given a legacy software and further extended it during their PhD until it did fit their needs. The purpose of this custom software was to produce publishable scientific results. The software itself was only a (unwanted) by-product. As such it was neither designed for maintainability nor well documented.

Even institutions that have an inhouse software or framework developed by a group of individual researchers suffer from such development practices. This has produced many rather unmaintainable software dinosaurs. They have a lot of hidden undocumented features unknown to current developers. This leads to new researchers reimplementing functionality that they need.

Often the developing institutions have a rather narrow application area for their software. Therefore it is almost impossible to use the software in a slightly different area as originally intended. This again leads to researchers having to reimplement the wheel if they want to switch the application area or even the underlying numerics.

This situation was a thorn in the eyes of the DUNE developers. At the time of DUNE’s inaugurating meeting 2002 they decided to attack these problems. The developers come from different institutions and have different (numerical) backgrounds. Quite a few of them had their own legacy inhouse software when DUNE started, at that time mostly grid managers. The purpose was to develop...
a unified interface to use them all underneath for different purposes. This interface should be slim. That is provide only absolutely necessary functionality. Nevertheless it should be universally applicable to different numerical methods. In contrast to many older interfaces it should be a fine grained interface in the sense that it is possible to access individual entries in a container (e.g. vertices of a computational grid or matrix entries) rather than just providing functions that work on the whole containers. Given the rise of modern C++ with templates this was possible without sacrificing computational efficiency.

2 The Development Cycle: History, Current and Future

It took approximately three years for fixing the initial interface and developing various prototypes. Some were full grids, others were based on legacy code but only exposed the interface of a DUNE grid. Another two years went by until we released the first stable version and published the papers [2, 1, 3] describing the interfaces.

Already at that time the DUNE community was divided into three groups: the so-called core developers that are allowed to vote on interface decisions, normal DUNE developers that have write access to the source code repositories, and other DUNE users that contribute with bug report and patches. This division exists until now. Active patch providers can become developers, if they find a core developer willing to mentor and take responsibility for them. A DUNE developer can become core developers with the support of the majority of the core developers.

Currently DUNE users play a more and more important role collaborating with the developers and we search for ways to raise their participation. This will be done with more regular user meetings. The first one was in 2010 and the next one will be in September 2013. This time there will also be a developer meeting directly afterwards. This will facilitate an even closer interaction between users and developers and make sure that future developments fit the need of an even more varied user base.

The main current aim is to establish a more foreseeable release cycle. We are planning to release roughly twice per year. This allows users to focus their own development on the current stable release and still be able to use most of the most recent features.

3 Key Sustainability Drivers of DUNE

3.1 Scientific Developers with Varied Backgrounds

The core developers of DUNE all come from various institutions, have different scientific backgrounds (e.g. Navier Stokes, linear elasticity, flow in porous media,
multigrid methods), and use different numerical methods. This makes sure that the software and its interface is usable for various numerical methods.

3.2 Open Source

From the beginning DUNE is available as open source. Its license is GPL-2 with the so-called “runtime exception”. This exception allows the template code of the DUNE modules to be used even in closed source projects. This was a prerequisite of some of the initial DUNE developers because there are German funding agencies that sponsor projects where both industry and academia collaborate. Currently there are big companies that adopted DUNE as their development platform due to its openness and even open sourced some of their own products.

3.3 Modularity

DUNE consists of various modules, each for its own purpose. Currently there are seven core modules supported by the DUNE community and two discretization modules developed by some DUNE developers. This lets users choose just the functionality that they need or want.

When moving from one monolithic source tree to various modules, each with its own source tree, the developers also implemented a rather elaborate build system on top of autoconf and automake. This makes it simple for users to create their own DUNE modules by simply calling a script. The new module now has the same build system support as the core DUNE modules and allows for code and build system reuse.

Today there are various other large frameworks based on DUNE: DUMUX, a framework for multi-physics, multi-phase, and multi-domain simulation, [4], and OPM, the open porous media initiative, [6], that strives to build an open source simulator suite for flow and transport in porous media for the oil industry.

3.4 Semi Open Development Model

The further development of DUNE is open. There are regular developer and user meetings. Even the developer meetings are open to others upon request. At the developer meetings important decisions, such as interface changes, are made. The core developer, currently nine from eight different institutions in Germany, the UK, and the USA, are able to vote during decisions and a majority of them is needed for a decision. Most decisions are discussed a priori on the mailing list or the bug tracker. Smaller once are even decided there. This procedure makes sure that only changes or additions are made that make sense to and are really needed by the majority. Flaws in an initial proposal are easily detected because of the diverse application areas of the developers and users.

In recent years the cooperation of the DUNE users with the DUNE development has increased. We receive various important bugfixes from them. Due to the stability of the development branch of DUNE experienced users often
choose to use it in their everyday work and development. This leads to many human testers and helps to further improve the stability of DUNE.

3.5 Code and Interface Reviews

Since the beginning DUNE was developed publically using modern version control systems (VCS): first subversion and since 2013 git. All committed patches are also send to a special mailing list. Most of the core DUNE developers read this list and thus review the patches. This often helps to detect bugs, possible problems with downstream user modules, or not aprooved interface changes very early in the development process. If developers want to change the interface, then they have to provide a proposal that has to be aprooved by the core developers at one of their meetings.

3.6 Joint Development by Industry and Academia

Since 2011 one the core developers has become an entrepreneur and is now providing DUNE contract work, and support. Commercial entities participating in the DUNE development naturally have a long term interest in the development. Often they have resources available for infrastructure work (e.g. build system, testing, and usability features) and naturally do quality management. This reduces the work for scientific developers and lets them focus more on the science side. In the end this will be advantageous for all.

References

[1] Peter Bastian, Markus Blatt, Andreas Dedner, Christian Engwer, Robert Klöfkorn, Ralf Kornhuber, Mario Ohlberger, and Oliver Sander. A generic grid interface for parallel and adaptive scientific computing. part II: implementation and test in DUNE. Computing, 82(2–3):121–138, 2008.

[2] Peter Bastian, Markus Blatt, Andreas Dedner, Christian Engwer, Robert Klöfkorn, Mario Ohlberger, and Oliver Sander. A generic grid interface for parallel and adaptive scientific computing. part I: abstract framework. Computing, 82(2–3):103–119, 2008.

[3] Markus Blatt and Peter Bastian. The iterative solver template library. In Bo Kagström, Erik Elmroth, Jack Dongarra, and Jerzy Waśniewski, editors, Applied Parallel Computing. State of the Art in Scientific Computing, volume 4699 of Lecture Notes in Computer Science, pages 666–675. Springer, 2007.

[4] DUMUX. http://www.dumux.org/.

[5] DUNE. http://www.dune-project.org/.

[6] OPM. http://www.opm-project.org/.