Cactus: Issues for Sustainable Simulation Software

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Abstract—The Cactus Framework is an open-source, modular, portable programming environment for the collaborative development and deployment of scientific applications using high-performance computing. Its roots reach back to 1996 at the National Center for Supercomputer Applications and the Albert Einstein Institute in Germany, where its development jumpstarted. Since then, the Cactus framework has witnessed major changes in hardware infrastructure as well as its own community. This paper describes its endurance through these past changes and, drawing upon lessons from its past, also discusses future challenges for Cactus.

Index Terms—frameworks, scientific computing, software sustainability

I. INTRODUCTION

Motivated by the needs of the numerical relativity research community and stemming from earlier efforts at the National Center for Supercomputer Applications in the U.S., the design and development of the Cactus framework [1], [2] began at the Albert Einstein Institute, a Max Planck Institute for Gravitational Physics in 1996. The component-based architecture of Cactus was inspired by experiences of physicists and computer scientists who had previously worked together in the USA Binary Black Hole Alliance Grand Challenge. This NSF-funded collaboration (1993-1999) involved over eleven groups, working with a variety of independent code bases on a set of different projects with the aim of modeling the inspiral collision of two black holes using then-state-of-the-art supercomputers 1. Even within a single group, multiple codes were used, often with multiple versions of each code. Contrary to the spirit of collaboration, advances in research methods or computing technologies were re-implemented, debugged, and verified in each code, thus duplicating effort, hampering communication, and slowing scientific progress.

The vision of the Cactus team was to provide an organic, community-oriented framework that would allow researchers to easily work together with reusable and extendable software elements.

From the beginning, the Cactus framework followed a completely modular design. It features a comparably small core (named the “flesh”) which provides the interfaces between modules at both compile- and run-time. The Cactus modules (called “thorns”) use these APIs to specify inter-module dependencies, e.g. to share or extend configuration information, to use common variables or run-time parameters. Modules compiled into an executable can remain dormant at run-time. Based on user-specified parameters and simulation data itself, the flesh decides when and in which order to call functions in different modules, assembling them into a coherent simulation.

This usage of modules and a common interface between them enables researchers to 1) easily use modules written by others without the need to understand all details of their implementation; 2) write their own modules without the need to change the source code of other parts of a simulation in the (supported) programming language of their choice; and 3) easily communicate the scientifically relevant ideas behind the module without involving the infrastructural details. The number of active modules within a typical Cactus simulation ranges from tens to hundreds and often has an extensive set of inter-module dependencies.

II. AN EVOLVING FRAMEWORK COMMUNITY

The accelerating growth and diversity of the Cactus community reinforced the modular development of both the physics-based and computational infrastructure. Examples of modules include the evolution equations for General Relativity, radiation or reflective boundary conditions, MPI parallelization, parameter parsing, and output routines. The value of this modularization is hard to overstate.

This design was of tremendous help to the motivating science problem, numerical relativity. It also became clear that with such a design, the modules could easily be purposed for other science problems. PDE problems are especially well-suited for use with the Cactus framework, however, since Cactus was initially written for numerical relativity, which solves a set of complex, partial differential equations (PDEs).

The straightforward reusability of existing components spurred development in other areas of science—usually numerically similar—in particular solving sets of PDEs, e.g.,

1The first accurate black hole inspiral was finally modeled in 2007.
coastal simulations of storm surges. However, most users of the Cactus framework by far are interested in numerical relativity, or more generally, relativistic astrophysics. Cactus development within this field is coordinated within the Einstein Toolkit [3, 4]. This focus stems, at least in part, from the fact that during most of Cactus development, interaction between developers and users was tight. In fact, most users became developers to some degree relatively quickly, so that users and developers were never truly distinct categories. One of the main reasons for this is the modular plug-in nature of Cactus, allowing end users to add new thorns to their application.

The majority of developers saw as their main motivation the pursuit of numerical relativity simulations rather than the broadening of the user base of the framework itself to other areas of science. However, owing to the modular nature of the framework, such a broadening was brought about as a result.

Today the Cactus and the Einstein Toolkit communities are still strongly interlinked through individuals who are active in both communities; but as different subdomains expand their usage of Cactus, these two groups polarize into different roles. Already, most users of the Einstein Toolkit are not active developers of the underlying framework itself, but rather merely use it to create and extend modules within the Einstein Toolkit, still occasionally contributing through new infrastructure; but their use of the framework informs the infrastructural developers’ priorities.

III. Software Sustainability Issues

There are many issues connected to the sustainability of software. Some of these are important for almost all software projects, but some aspects are especially relevant for scientific projects. Out of the latter the authors picked four of the most relevant to discuss in more detail.

A. Modular Design

One of the key properties of a long-term sustainable scientific software is a modular design. Cactus chose a unique method of enabling modularity that went beyond the usual notions of APIs, standard data structures, and coding conventions. Cactus uses a small set of domain specific languages (DSLs) to describe its distributed data structures and scheduling [5]. These DSLs enable Cactus modules to do run-time reflection, in both Fortran and C/C++, on the grid variables being evolved.

This may not sound like a revolutionary idea, but its consequences were far-reaching. Because of this simple design decision, several things became possible. First, Cactus was able to completely decouple I/O from science code. Unlike many scientific codes that have calls to I/O routines interspersed with the program logic, science modules in Cactus are only concerned with what variables they read and write. The I/O module(s) can take field variable names as a parameter, look them up with run-time reflection, and write them out as text, HDF5, JPEG and other formats. The DSL describing scheduling identifies when this I/O will be performed, steered at start or even run-time by the user. Even the most important form of I/O, checkpoint/restart, is enabled and modularized by this design.

Second, Cactus was able to abstract the time-integration method (e.g. Runge-Kutta, Iterative Crank-Nicholson, etc.) from the time evolution equations. The DSL describing scheduling, combined with the list of variables to be evolved, was sufficient for this task. The value of this module by itself is significant. The ability to avoid subtle coding bugs or to try out diverse integrators, without cluttering the codebase, is of great value. This time integration module can also easily be used to couple separate physics modules, such as e.g. the Einstein and Hydrodynamics equations.

Third, Cactus was able to create a web browser interface, interrupting the schedule tree at key places and allowing variables to be inspected and modified during an execution. This particular form of parameter steering was naturally enabled by the key module design decisions.

Fourth, an adaptive mesh refinement module named Carpet [6, 7] was added. Before Carpet was available, only uniform, Cartesian grids could be used for spatial decomposition within Cactus, and a lot of modules expected to get such rectangular meshes as input. It was possible to integrate Carpet into Cactus without almost any change to the science modules. Later, a multi-block mesh capability [8] was added with similarly little disruption to existing codes.

There are many other capabilities enabled by the unique modularization decisions of the Cactus Framework. Other special modules include those for debugging, e.g. NaNChecker, those enabling unusual IO, e.g. Twitter, generic grid modules, generic boundary conditions, timers, interfaces to PAPI counters, analysis modules, etc.

These unique types of interfaces allow different groups to efficiently work on one common project, towards one common goal, avoiding unnecessary conflicts or duplication.

B. Growing Collaborative Community

In contrast to commercial products, academic scientific software like Cactus is usually developed in a university setting. Most of the actual development work is performed by graduate students and postdoctoral researchers who are focused on science. This poses a threat for long-term stability of any project, because these developers are typically not very interested in contributing to infrastructure, and frequently leave their research groups after three to four years, taking all their knowledge and experience with them. New members of research groups first need to be trained, and while this time can be shortened by creating
respective courses and documentation, e.g., [9]-[11], the constant flux of developers continues to be a struggle.

The infrastructure development problem is handled within the Cactus community by connecting its development so closely to a specific science problem that publications that describe both are possible. This is the way many of the publications using and extending the Einstein Toolkit are written, containing a description of the new infrastructure while mainly representing a publication in physics. On the other hand there are examples of pure computational science publications as well, e.g., [12]-[17]. These sorts of projects are enabled by the ability to provide immediate benefits for the substantial number of physics problems described by the Einstein Toolkit.

The retention problem is handled by the Cactus community automatically, by creating an enjoyable programming and development experience. Many students continue to be interested in and develop for Cactus after they move on to new positions. They are attracted by the ability to leverage the work of other physicists and computer scientists in the community, to see their code re-used, and to collaborate on new research. The ability of Cactus to enable collaboration, based on its unique modular design and the use of open-source licensing, make it an attractive tool for students to use in their continuing research. Thus, rather than really leaving, they expand the collaboration. Not all students continue to use Cactus, but enough are inspired by it to create the kind of stable contributions needed to maintain the health of the project.

C. Career paths

The third issue connects to the main motivation of the workforce as well, but also affects the group leaders, especially if they are young faculty or trying to become faculty. In contrast to commercial products a main motivation of developers in academia is credit. Credit is obtained through publications and citations thereof, which are then used to quantify the scientific impact of an individual’s work, forming the basis for future career plans as well as promotion and tenure for faculty. The most severe problem for developers in most computational sciences currently is that while most of the work is done creating hopefully well-written, sustainable software, the academic success is often exclusively tied to the solution of the scientific problem the software was designed for. Tasks that from a software engineering standpoint are essential, e.g., high usability, well-written and updated documentation, or porting infrastructure to new platforms, are not rewarded within this system.

While computations of some form entered almost every aspect of academic research and have been present in many areas already for years, criteria for tenure positions especially often rate scientific results much higher than the infrastructural development that was necessary to achieve these results. Developers of scientific software are often experts across disciplines, and thus very valuable as a team member, group leader and lecturer. However, the scope of open tenure positions is often only very limited to a specific traditional science, resulting in a lack of career opportunities and thus a lack of student motivation to fully participate in these cross-discipline activities.

D. Credit

All the previously mentioned ways to publish assume these papers are cited when the described software is used by others. While this is often the case, it is also not uncommon that relevant citations are missing despite the usage of a specific software package. Enforcement of citation is hard to impossible to enforce especially for open-source software like the Cactus framework. Any requirement for citation would conflict with its free-software license. Changing the license on the other hand, e.g., to include such a requirement, is also not desired, because there are legitimate cases where such citations are not possible, e.g., because of space limitations.

Both the Cactus framework and its largest user group, the Einstein Toolkit, have a few general publications that are requested (but not required) to be cited whenever the software is used, and especially the Einstein Toolkit also requests additional citations when some of its modules are used that are so complex that they are described in publications of their own and deserve extra credit. Examples of such modules are the Carpet mesh-refinement infrastructure, or the black hole horizon finder [18]. Handling citations on a module-level like this enabled individual developers to receive credit for their work, especially if they entered the group only after the main publications had already been written. A complete list of these publications can be found on the Einstein Toolkit web site [4].

IV. Future Challenges

Computational science is always evolving, and at an ever increasing pace. Changes in hardware and progress in numerical methods have been important factors in the quest to solve increasingly complex problems within a relatively constant time. The Cactus group is looking for ways to use modularization to attack these new types of problems.

Prior to the discovery of a stable set of numerical techniques for evolving black holes, it was necessary to experiment with the form of the Einstein equations. Unfortunately, these equations contain many hundreds of terms and transforming them into code was daunting, tedious and error-prone. Sascha Husa and Ian Hinder developed a tool called Kranc [19], [20] to mitigate this problem. Kranc takes a tensorial equation written in Mathematica and generates a complete Cactus module in C++ to evaluate it, enabling scientists to more easily experiment with the form of equations. Kranc turned out to be a much more powerful and useful tool than anticipated.

Modern architectures increasingly rely on vectorization to achieve performance, many of them now performing
eight floating point instructions per clock cycle. Unfortunately, few compilers can vectorize the Einstein equations because of the sheer number of terms they contain, leading to a large performance penalty.

Recent work shows that Mathematica’s pattern matching ability allows us to transform equations as Kranc generates them, generating explicit vector instructions and side-stepping compiler limitations.

Kranc provides another mechanism and opportunity for modularization. Because it isolates the high level representation of the equations from their implementation in code, it makes it possible to generate code for multiple languages (such as CUDA, and OpenCL), and for multiple numerical methods as well (e.g. Discontinuous Galerkin, finite differencing, etc.).

Thus, equation generation provides a possible path forward for increased modularization and functionality for the Cactus framework.

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