developing scientific software......

Development of a Weather Forecasting Code: A Case Study

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A case study of a weather-forecasting code aimed to investigate the code development challenges, understand the development tools used, and document the findings for other developers. omputational science is increasingly providing insight into scientific phenomena that have previously been studied only experimentally, observationally, or theoretically. Codes, the software projects written for computational science, generally have three main differences from traditional software projects, such as those from the commercial software domain. First, because these projects often perform new scientific investigations, the requirements can't be known in advance and must evolve over time. Second, the main driving force for these projects is producing correct,

important scientific advances rather than ensuring software quality through formalized software engineering processes. Finally, these projects' developers tend to be domain scientists rather than software engineers, so they're less likely to use any heavy software development processes.^{1–3}

To better understand the impact these characteristics have on software development practices in the computational-science domain and to document lessons learned for similar projects' benefit, we performed a series of case studies of computationalscience code development projects sponsored by the DARPA High Productivity Computing Systems program. Here, we describe the sixth case study (after Falcon,⁴ Hawk,⁵ Condor,⁶ Eagle,⁷ and Nene⁸).

The common objectives for all case studies were

■ identifying critical success factors,

- identifying issues that hardware and software vendors must address to make the code development process more productive,
- developing a reference body of case studies for the computational science and engineering community, and
- documenting the lessons learned from analysis and personal team interviews.

For this case study, we followed the same methodology that we used in the previous case studies.² Here, we provide only a basic overview of the methodology to give context for understanding the results. After we identified a suitable project, the team completed a questionnaire. We used the responses to plan an on-site interview, after which we iterated the results with the code team to ensure correctness.

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Code characteristics

Osprey is one component of a large weatherforecasting suite that combines the interactions of large-scale atmospheric models with large-scale oceanographic models. Osprey's current codewhich has evolved from other codes that date back to 1974-has been used operationally for 10 years. Development of the present version began in 1988 as a research project that aimed to extend the predecessor code's capabilities. At the highest level, the Osprey code team has some control over the requirements through the proposal process. That is, the team can make direct proposals to potential sponsors about features to implement in the code. This process is how the team acquired funding for code-directed goals such as the implementation of the Message Passing Interface (MPI) and nested grids. The sponsors, which have increased in number in recent years, often set the requirements through directed research and development grants (that is, unsolicited grants). Work tends to be funded in ever-smaller increments (relative to constant costs), and individual code developers now work in multiple topic areas rather than specializing in one topic.

Osprey is distributed via the Web. It has no license fee, and the team has deployed a home-grown license manager to track the code's distribution. Osprey has been downloaded hundreds of times by institutions worldwide. Some institutions have hundreds of users.

Because the Osprey code is one component in a larger system of systems, its architecture lets it both send and receive information from the other system components. A framework supports one-way and two-way coupling of Osprey to other system components, using an exchange grid to facilitate data exchanges between components.

With the exception of approximately 300 lines of C code, Osprey is written in a Fortran subset (which we describe in the next section). There are approximately 150 KLOC in Fortran, of which approximately 50 KLOC are comments. The driving motivation behind choosing Fortran was the need for portability and ease of development and maintenance (similar to our findings in the Falcon, Condor, and Nene case studies). After considering these needs, Osprey determined that Fortran was the best language available when development began. Although university computer science departments no longer routinely teach Fortran, new developers can master its fundamentals in a week (using Fortran 77) to a few months (Fortran 90). In contrast, C++ or other modern, higher-level languages typically take much longer to master. Furthermore, using an all-Fortran code eliminates complicated **moke** and link operations and other problems associated with using multiple programming languages. The project leader hasn't encountered any limitations in Fortran (augmented with the MPI) that would cause him to seriously reconsider the choice. Moreover, programminglanguage evaluation has been a distraction in the past, so the team is reluctant to invest resources in this area unless it has identified a specific need, such as the one that led to implementing MPI.

Essentially one version of the Osprey program library executes on SGI, IBM, HP, and Linux platforms. A locally built preprocessor configures the code for each supported platform. Compiler flags configure the code to run using different parallel-programming libraries (such as MPI and OpenMP).

Parallelization is a key priority because the team must use parallel computation and processing to achieve the performance level needed to obtain the expected scientific results. Conversely, actual demonstrations of parallel performance haven't reached the level that the Osprey development team believes is feasible. This shortfall results from the fact that, to maintain portability, the code isn't highly tuned for any specific parallel platform; however, some optimization occurs for each platform. In general, however, the team avoids the use of libraries and machine-dependent features. Earlier attempts at hardware-based customization led to cluttered, unmanageable code. The emphasis now is on general, flexible, and scalable code.

Code project and team

Osprey's core team consists of about 10 developers and a few outside consultants and postdoctoral researchers. The core team is located at a single site along with most of the development teams for the other components in the larger system of systems. However, other sites also contribute components. Most of the core team members have worked together for the past 10 years. The team leaders have preferred to recruit staff members who already have domain knowledge. Moreover, the team has generally found individuals with computer science backgrounds to be helpful for specific coding tasks or applications, but it hasn't utilized computer scientists as part of the primary code development team. The team has had difficulties interfacing with pure computer scientists that have had little exposure to large weather or oceanography codes. As an example of the difficulties the team has experienced working with computer scientists, the Osprey team leader cited

a computer scientist who wanted to make every executable line of the code into a subroutine to make the code easier to debug.

The Osprey team describes itself as follows:

- Team members have a common professional background.
- Team management processes are largely informal and collegial.
- There is strong peer pressure to contribute and strong team member dedication to the project.
- The team views code validation as especially important.

The Osprey team indicated that code maintenance, portability, and speed-to-solution are the main drivers of development, with ease of maintenance being paramount. They also emphasized flexibility, by which they mean

- the code must run on many platforms,
- the code must port easily to the next generation of hardware, and
- the code can't be tailored to any particular platform.

This definition of flexibility represents a conscious attempt to manage an important technological risk. The Osprey developers aren't encouraged to use all of the constructs that Fortran supports. The practice within the Osprey development community is to use only features that are well tested and reliable. The team follows a style guide and uses the structure and coding practices of the code itself to train new team members.

Osprey and the developers of the other systemof-systems components are colocated and under a common management structure. This colocation, along with the Osprey development team's relatively small size, has limited the degree of formality needed to manage the team. The Osprey team doesn't adhere to any formal code development methodology (such as CMM, ISO, or even formal agile development processes). However, the team has adopted repeatable coding practices and employs coding-style requirements and standards. From the formal software engineering viewpoint, this project is underconstrained-as have been all but one of the other computational science projects that our team has examined in case studies. This approach is successful because, for the most part, the Osprey team can set its own milestones with the sponsors' approval; thus, the iron triangle (that is, the scope, resources, and schedule) isn't violated. Although the team doesn't identify with formal development processes, it follows an agile philosophical approach (www.agilealliance.com) in the sense that it emphasizes practices over process. Table 1 summarizes the extent to which the Osprey team uses various development practices.

Of the 20 or so software development tracking metrics⁹ cited in the software engineering literature, the Osprey team employed

- lines of code,
- code performance,
- degree of performance optimization,
- parallel scaling,
- number of users, and
- computer time used for code development.

LOC is a general measure of the code's growth. There is growing pressure from sponsors for science metrics, not code development metrics.

Osprey's approach to configuration management is similar to that of the other projects we've studied. A part-time source code librarian uses Subversion (http://subversion.tigris.org) to manage the code. The code librarian logs the bugs. No formal issue-tracking system has been deployed, nor does one appear to be necessary. The code librarian requires a prologue detailing a subroutine's purpose before it can be committed to the code library. Verification tests are also required.

Code life cycle and workflow management

Much of the Osprey program library's code is in maintenance. Because Osprey is undergoing continuous enhancement, there's always new development and testing. At any given time, code modules in the program library range from brand new to 20 years old. This project's workflow is typical of the other projects that we've studied, consisting of the following steps:

- question formulation,
- development approach formulation,
 - code development,
 - testing (validation and verification),
 - production,
- analysis, and
- hypothesis formulation.

(This isn't customary software engineering language—such as requirements gathering or specifications formulation—but it's more descriptive of the actual workflow management process the computational-science projects we studied employed.)



Table 1The Osprey team's development practices

Practice	Description	Followed	Comments
Collective ownership	Allow anyone to change any code anywhere in the system at any time.	Partially	Followed to a small degree; a limited set of developers allowed to make changes
Configuration management	Establish and maintain the integrity of work products using configuration identification and control.	Yes	A key role in this project
Continuous integration	Integrate and build the system many times a day, each time a task is completed.	Partially	Performed weekly rather than daily
Feature-driven development	Establish an overall architecture and feature list, then design by feature and build by feature.	Yes	Project development driven by new features
Frequent delivery/ small releases	Have many releases with short time spans; implement the highest-priority functions first.	No	Driven by task—no explicit goal to have small releases, although this often occurs
Onsite customer	Include a real, live user on the team who is available full time to answer questions.	Yes	Code's developers are also users
Organizational process definition	Follow an organization-wide process.	No	No formal organization-wide process
Organizational training	Develop team members' skills and knowledge so that they can perform their roles effectively.	No	Nothing formal in place
Pair programming	Work side by side with another programmer at one computer, collaborating on the design, algorithm, and code.	No	Not found to be useful
Planning game	Quickly determine the scope of the next release with business priorities and technical estimates.	No	Not used
Peer reviews	Review peers' software artifacts (requirements, design, code) to improve quality.	Partially	Informal code reviews (but not requirements or designs) used
Process and product quality assurance	Objectively evaluate adherence to process descriptions and resolve noncompliance.	Partially	Long-term roadmap for Osprey, but no formal monitoring of adherence to the development strategy
Project monitoring and control	Provide an understanding of the project's progress so that appropriate corrective actions can be taken if progress deviates from plan.	Yes	Internal and external reviews throughout the year; local groups meeting weekly to discuss issues
Project planning	Establish and maintain plans that define project activities.	Yes	Planning done at the beginning of each fiscal year as part of the funding cycle
Refactoring	Restructure software to remove duplication, improve communication, simplify, or add flexibility.	Yes	Used to improve performance and make it easier to change the code in the future
Requirements development	Produce, analyze, and verify customer, project, and product requirements.	Yes	A formal process followed as part of proposal generation
Requirements management	Manage the project's requirements and identify inconsistencies with the project plan.	Yes	Internal milestones set by each subteam
Retrospective	Perform a postiteration review of the effectiveness of the work performed, methods used, and estimates.	Yes	Performed at the annual review
Risk management	Identify potential problems and adequately handle them.	Partially	Emphasis on testing and benchmarking; conscious strategy for managing technology risks; no formal management of other risks
Simple design	Design only what is being developed, with little planning for the future.	Partially	There's a long-term plan beyond the current funding; the design is documented only in the code, so features that aren't coded haven't been formally designed
Tacit knowledge	Maintain and update project knowledge in participants' heads rather than in documents.	Yes	Tacit knowledge in the scientific discipline is important
Test-driven development	Write module or method tests before and during coding.	Partially	Testing integrated with development

The development path through these steps is iterative. The team developed physics prototypes for testing in the Osprey code framework. The team wrote these prototypes as candidates for direct inclusion into the code, so there's also an aspect of spiral development. Unlike some other projects we've studied, these prototypes aren't written in a higher-level language such as Matlab. However, the Osprey team sometimes uses Matlab to study parameterization issues. There is some refactoring of old modules as capabilities are replaced or enhanced. The project has no mandated release schedule; releases occur when new capabilities or bug fixes are ready. Last year there were 10 releases, but some were small fixes. The downloadable version is two years old (that is, well behind the most current version).

As we've observed in our other case studies, most sponsors don't directly fund code maintenance. It's not entirely clear that development is funded directly either—the funding is usually directed toward the science, not the code.

The team does testing both during and at the end of development. Team members can't submit new capabilities for inclusion in the Osprey program library unless the capabilities pass verification tests. The developers do substantial testing before submitting capabilities to the configurationmanagement process. Team members share quality assurance. After internal testing, the code is transferred to a primary customer for additional, independent testing prior to release. For major changes, an independent panel with broad stakeholder representation performs a series of tests before the transition to production.

A goal of our case studies has been to document the tools the code development teams use (see Figure 1 for a summary of these for Osprey). The use of particular tools, such as TotalView, hasn't been mandated and is often a matter of personal preference. IDL is used primarily by customers, not developers. In general, developers prefer open source tools.

Lessons learned

All our case studies have extracted important lessons for the computational science and engineering code development community. These lessons can guide software engineers seeking to better understand how to successfully work with this type of code project. In this case study, we present two types of lessons learned. First, we describe the lessons the Osprey team members learned. Then we combine those lessons with our observations from the questionnaire and interviews into the context



of our previous studies' findings.

Figure I. Osprey's life-cycle management tools.

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- If it's important, do it right.

following lessons learned:

- Listen to the customer.
- Data assimilation becomes increasingly important as the model grows in sophistication.

First, the Osprey team members articulated the

- Configuration management is essential.
- Physical parameterizations remain a necessary evil, but you should avoid them if physical models are feasible.
- Validation and verification are crucial to improving and accepting scientific codes.
- Strive for performance, but not at all costs.
- Build flexibility into the system.

In our previous case studies of computational science codes, we made nine observations about the software development environments used.² The lessons the Osprey team learned and our observations from the questionnaire and interviews provided support for seven of those earlier observations. Here, we describe them in more detail along with the supporting information from the case study.

A code project's primary language is constant over the project's long lifetime

These projects tend to last multiple years (even decades), as evidenced by the fact that some of the Osprey project's code dates back 30 years. Therefore, you might expect that the programming language would evolve over time as more modern languages are developed and standardized. Conversely, in Osprey and the other codes we studied, the basic language didn't change over time. The The Osprey team still uses Fortran because it's easy to learn compared with modern languages. Osprey team still uses Fortran because it's easy to learn compared with modern languages. This is true also because the team has yet to encounter a weather-modeling requirement that couldn't be programmed efficiently, both in terms of programmer effort and execution time, using Fortran.

Use of higher-level languages is low

The Osprey project uses high-level languages such as Matlab very sparingly, if at all. In some other cases, we've seen Matlab used as a prototyping language almost akin to a statement of requirements. But none of the projects we studied extensively used such languages.

Risk management is important

These types of projects' long lives present risks that aren't always present in other types of software. In our previous studies, teams viewed externally developed tools and libraries as risky because of the likelihood of the vendor going out of business during the project's life cycle. For the Osprey project, lack of flexibility was an important risk. To address this risk, they designed and implemented the code so that it wasn't closely tied to any particular platform and could be easily ported to new platforms as they became available.

Performance isn't the only important nonfunctional requirement

All the code projects we studied used highperformance supercomputers, so performance (that is, speed of execution) was an implied goal. In Osprey, performance is an important goal, but only to the extent that it improves the code's scientific output. In other words, scientific goals drive the need to achieve a particular performance level. Osprey's main focus is to support scientific research, not to demonstrate computer science ability or even achieve impressive performance numbers. Although it isn't the main driver, code performance is still important to the Osprey team because its customers require real-time applications that support operational functions. In addition, as discussed earlier, maintainability and portability are also essential to the Osprey code's success.

Agile approaches are better suited than more traditional methodologies

In the projects we studied, including Osprey, scientific-code teams valued agility over formalized processes. That is, they usually avoided rigid software management approaches, but planning and adoption of useful software practices *are* important to the success of these projects. We've found that

development teams can function well with a very lightweight process as long as teams are small, perform adequate planning, and have good communication among team members. Although Osprey and the other code teams we studied didn't use one of the formal agile methodologies (such as Scrum or XP), they did operate their team according to the mind-set proposed in the Agile Manifesto (http:// agilemanifesto.org). The choice to operate this way emerged out of necessity rather than a conscious decision to follow one specific agile approach over another.

Multidisciplinary teams are important

The complex nature of the scientific domains for which computational science is effective necessitate that much of the code be written by domain experts (scientists). It's simply too difficult to teach a computer scientist or software engineer the technical details of a scientific domain for which a PhD is needed to even understand the problem to be solved. In many cases, including Osprey, these teams have found it effective to use computer scientists' expertise and ability to perform specific coding tasks that don't require extensive domain knowledge.

Project success or failure depends on keeping customers and sponsors happy

As in any type of project, its longevity depends on its success among its customers. One unique aspect of the computational science projects we studied, including Osprey, is that the customer and the users aren't always the same group of people. So, to be successful, a project must keep both the users (other scientists) and the customers (the sponsors or funding agencies) satisfied. If the code project meets the technical goals the customers set, but isn't seen as useful by the end users, then it won't be viewed as a success over the long term.

e hope that these lessons learned will be useful to other scientific-code developers. We realize that the Osprey project might be unique and might not represent experiences in other domains. Nonetheless, we believe that many of these lessons are applicable to a broad range of computational science projects.

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Osprey is a pseudonym; we have masked or omitted any details that might reveal the code project's identity.

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