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Experiences from Software Engineering of Large Scale AMR Multiphysics Code Frameworks

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1 Introduction

Among the present generation of multiphysics HPC simulation codes there are many that are built upon general infrastructural frameworks. This is especially true of the codes that make use of structured adaptive mesh refinement (SAMR) because of unique demands placed on the housekeeping aspects of the code. They have varying degrees of abstractions between the infrastructure such as mesh management and IO and the numerics of the physics solvers. In this report we summarize the experiences and lessons learned from two of such major software efforts, FLASH [1] and Chombo [2].

Both Chombo and FLASH are built on top of the same SAMR principles, however, their purpose and reach are very different. Chombo is primarily an AMR framework that comes with built in solver technologies. Typical Chombo users build application codes for their domains by treating Chombo as a toolbox. Therefore, Chombo has been the basis of such application codes as Bisicles, ChomboCrunch, Compass and several others. FLASH, on the other hand, is a complete application code that can use Chombo as one of its mesh packages. The greater emphasis in FLASH development is on the physics modeling capabilities. Typical FLASH users combine vast majority of capabilities provided by the code in different ways, customize some of them and/or add relatively small amount of code of their own. Chombo expects its sophisticated users to modify some of its lower levels, FLASH takes a great deal of trouble to avoid such occurrences. Because of these differences in approach there are differences in the designs of the two codes, however, there are many more similarities in their software engineering and process than there are differences.

2 Software Engineering

FLASH started its life as an amalgamation of three independent codes written predominantly in f77 style. From the beginning the principle purpose was to be able to simulate phenomenon of scientific interest at the earliest possible opportunity. The architecture and modularity was achieved by unraveling the data structures and lateral dependencies over several iterations. Chombo, on the other hand, started as not-backward-compatible branch of the BoxLib Framework, a collection of tools to manage adaptive mesh. The reason for this bifurcation was to serve the divergent needs of two groups using Boxlib as their basic source. The Chombo team made significant changes to the API layers above Boxlib that were best suited for their own purposes. The other major difference that influenced the design of the two codes was the language. Chombo had the advantage
of language supported object oriented features, while FLASH imposed its own object oriented approach on non-object-oriented code kernels through the use of unix directory structure and a limited domain-specific-language (DSL) for configuration. This difference is reflected in ways that encapsulation and abstractions play out in the two codes.

However, the maintenance process is very similar in both codes. They use subversion for version control, have well defined coding standards and ongoing verification practices. Both the codes have been largely successful in realizing the separation of concerns between the numerical and parallel complexity of the codes through modularization and adoption of component based architectures. The abstractions and modularizations are usually accompanied by some reduction in the overall performance of the code. Also, given the relatively short shelf life of computing platforms and the large source bases that these codes have, portability is an ongoing priority. The judicious trade-off between maintainability, portability and performance has been the hallmark of these and many other successful SAMR and other multiphysics codes. The most important area of similarity between the codes is that they both had long term sustained funding in the initial stages to devote to code infrastructure. Resources could be allocated for designing the code architecture and the appropriate mechanisms for ongoing code maintenance and verification. The current lack of such sustained funding is a big threat to these and other large codes in similar circumstances.

3 Lessons Learned

The following are the combined lessons learned by the two code teams that might be of interest to other projects at similar scales.

**Public Releases**: Early and frequent public releases of the code are greatly beneficial to the overall code quality. The general tendency to keep the code private for perceived advantage over the scientific competition is misplaced and often detrimental to both code and science. Early and relatively frequent releases serve the dual purpose of ensuring that the coding standards are followed more carefully and that code verification is broader because of being exercised in many different ways by diverse users. Public releases also facilitate the reproducibility of science results and therefore confidence in those results.

**Interdisciplinary Team**: A team with a breadth of knowledge and expertise is compulsory almost by the definition of the work involved. There must be domain experts as well as applied mathematicians and software engineers in the team. At least a couple of team members should have cross-cutting expertise. This is useful not only in terms of understanding how the various components work together in the software, but the presence of such individuals also fosters trust and co-operation among the diverse team members. A team with broad and cross-cutting expertise is also able to better absorb the loss of individuals with specific expertise.

**Documentation**: Extensive documentation is critical not only for the user population, but also internally for code maintenance. In addition to standard documentation such as a user’s guide and other online resources targeted at the users, extensive inline documentation is critical for maintaining any code section that has even moderately complex logic. A well documented code section can be maintained by non-experts with general know-how of the code if necessary. **Backward Compatibility** Our experience has been that backward compatibility is not always desirable during major version changes. It can get unnecessarily expensive in terms of developer time and can clutter the code architecture. There are several precedents for breaking backward compatibility to the advantage of the longevity of the code. This is especially true if a significant
API change is desired, and if the branch has adequate support to be a live project in its own right. Caution should be exercised in doing this for under-resourced branches because they may end up as nothing more than software research. That is not a bad thing, but it should be expected and planned for.

**User Support** Having a well defined user support policy is extremely important in convincing the community to use the code. While it may take significant resources initially to respond to all user queries, in time that effort reduces because the community becomes self-supporting. Providing comprehensive documentation which is easy to access and reference also helps reduce the demands for user support.

**Code Infrastructure** The least cluttered code architecture provides the greatest flexibility and longevity. While it may seem like stating the obvious, scientific codes very often fail to achieve this for several reasons. The most common reason is feature creep: almost all codes have features that should have been pruned because they either did not prove to be useful, or outlived their usefulness. Another common reason is that the code infrastructure is often erroneously assumed to be less important than capability development, especially when resource allocation is driven by near term scientific goals. The most important reason, however, is that it is extremely hard to achieve architectural simplicity in a complex software with many moving parts. It requires substantial investment on the part of the developers to understand the requirements, the limitations, and the idiosyncrasies of the core solvers as they relate to the infrastructure. The best time to devise and formalize code architecture is after the knowledge about the core solvers has been thoroughly internalized, and that requires a willingness to redesign and rewrite large chunks of infrastructure code at least in the early iterations.

Verification: Code verification in general gets some attention from scientific code developers, but ongoing daily testing usually does not. Any large development effort cannot have confidence in the code without such testing. Developers cannot comprehensively test for unintended side effects from code modifications manually when the code has many interoperating components. When there is daily testing with sufficient code coverage, chances of early detection of unintended side effects increases. The amount of effort needed to fix such inadvertently introduced faults is higher the longer they stay undetected.

4 Future Sustainability

In the era of cluster computing with fat nodes, distributed memory computing provided a near ideal programming model where these sometimes conflicting requirements of performance, portability and maintainability could be balanced. The overheads of communication primitives and bulk synchronizations could be amortized over large computational units to the point where they did not significantly compromise performance. Also, since the node architectures were mostly homogeneous even across vendors, general algorithmic or data structure optimizations provided benefits across the board. Therefore, although individual codes followed different paths, and differ significantly in their details, they have arrived at remarkably similar solutions conceptually. They are in production in multiple disciplines, are prolific in producing scientific results, and are likely to continue to do so for the next couple of years. This state of affairs combined with the uncertainty in the HPC landscape at present has induced hesitancy in prioritizing the infrastructure building in many code projects and their funding agencies. We believe that this could potentially be a recipe for disaster as more heterogeneous and less reliable machines come online.
The most frequently given argument that the code developers will rewrite their codes for the target platforms is a valid one for software with relatively small code bases. When the algorithms are well understood, and refactoring the code is likely to take only a few person-months there is nothing to be gained by anticipating trouble and preparing for it ahead of time. However, large code bases do not have this luxury. Some of them are likely to take several person-years to transform the whole code base. Our experience indicates that starting from scratch to write a whole new code is worse because of higher number of degrees of freedom for error introduction. It is our position that redesign and re-architecting of code frameworks does not need to wait for the arrival of manycore and heterogeneous platforms, because a consensus is beginning to emerge about the conceptual design requirements, enough to enable the redesign phase to start.

The emerging paradigms for taking the codes to the next generation include automatic code transformation and asynchronous runtime management. While the individual tools and compilers for providing these functionality will be different, the applications will have to provide footholds for the related abstractions. The applications can do so by taking the separation of concerns a step further than that between numerical and parallel complexity. They have to articulate the dependencies within the code much more explicitly, leave data-staging and therefore assembly to the infrastructure and expose minimum computation units, both spatial and temporal, that can be exploited by the code transformation tools through fusion.

Because of the above considerations, the refactorization and transformations are needed at the more fundamental implementation design level in the application codes and/or their infrastructure. The data layout, the wrapper layers and the communication channels between different code components have to be designed with an awareness of the semantics of the programming abstractions using asynchronous task management and code transformations. It is imperative that support is provided for refactoring of the mature codes in this manner because the changes to the architecture of most codes will be highly disruptive and therefore labor intensive. The alternative, code development from scratch, might succeed in a few instances, but is unlikely to meet with broad success. The reasons are: (1) an unconstrained design space has a potential to not converge, as happened to many high level frameworks 12-15 years ago, (2) code verification during refactoring remains tractable when solutions can be compared against a known set of solvers, and (3) to build a robust multiphysics code is long and arduous process, most mature codes have taken 5-8 years to arrive at the level of confidence that they now enjoy. We believe a judicious combination of disruptive and incremental changes are the optimal way to continue to serve the cause of science.

References

