Best practices for the procurement process of high performance computers by the Federal government

R. Scott Studham
Technical Group Leader
MSCFO - PNNL
P.O. Box 999
MSIN: K8-91
Richland WA 99352
+1-509-376-8430
studham@pnl.gov

Arthur S. Bland
Director of Operations
ORNL Center for Computational Sciences
P.O. Box 2008
Oak Ridge, TN 37831-6203
+1-865-576-6727
BlandAS@ornl.gov

William T.C. Kramer
Head of High Performance Computing and General Manager National Energy Research Scientific Computing Center (NERSC) - LBNL
MS 50B-4230
Berkeley CA, 94720
(510) 486-7577
kramer@nersc.

Robin Goldstone
Group Leader, Production Linux Group
LLNL
7000 East Ave. L-073
Livermore, CA 94550
(925) 422-5832
robing@llnl.gov

Cheryl Wampler
Group Leader,
CCN-7 LANL
High Performance Computing Systems
MS T084
Los Alamos, New Mexico 87544
(505) 667-0147
clw@lanl.gov

David A. Dixon
Battelle Fellow
Pacific Northwest National Laboratory,
P.O. Box 999/MS K9-90,
Richland, WA 99352,
509-372-4999
david.dixon@pnl.gov

Bob Ayars
Deputy Group Leader, CCN-7 LANL
High Performance Computing Systems
MS T084
Los Alamos, New Mexico 87544
(505) 667-9047
rsa@lanl.gov

This white paper is being submitted in response to question #8: "As input to HECRFT charge (3) overall, please provide information about how the Federal government can improve the process of procuring HEC systems and tools." The institutions and agencies represented by the authors have been involved in platform procurements of various sizes and natures, including some of the largest HEC platform procurements conducted by U.S. agencies, such as the Cray T3E system at NERSC, the IBM Power 3 and Power 4 systems at NERSC, ORNL, and LLNL, the Cray X1 at ORNL, the compaq HPQ system at LANL, the IBM Power 5 and Blue Gene systems at LLNL, and the large HP Linux cluster at PNNL. Different procurement methods have been used, including: (1) System specification based procurement, (2) Science driven (Greenbook) procurement with design criteria, (3) Performance driven procurement based on benchmarks of actual applications, and (4) Direct partnerships with industry. Often the actual procurement process is a combination of these methods. In all cases, it is critical that the eventual end-users and stakeholder of the systems play a role in defining specifications and requirements for the system and when feasible, participate in the procurement, integration, and evaluation processes.

In today's environment, clusters of symmetric multi-processor (SMP) computers are the most common choice to build a high-end computer system. The monolithic architectures such as the Cray computers that dominated the 1980s and early 1990s are no longer prevalent. Each new system pushes the previous limits in scale and represents a breakthrough in technology, requiring innovation and development to integrate the system. In order to accomplish mission objectives, i.e., advance the solution of complex scientific and engineering problems through the use of simulation, at minimum cost and maximize the overall system value, it is necessary to stay at the leading edge of the performance/price curve reflected in Moore's Law. Thus, it is very common at this scale that HEC procurements are for systems and technologies that do not exist

at the time of the procurement evaluation or contract signing. In all cases, there are tradeoffs between the length of time for the procurement, the costs involved both for the vendor and the procuring institution, the performance levels, the solution costs, the reliability of the system, and the risks of not getting what is contracted for. In view of the rapidly evolving nature of this field, the procurement and contracting process needs to be flexible and adapt readily to changes in technology directions in order to be successful. This white paper focuses on two of the primary procurement methods: (1) Technology-driven procurements, and (2) Science driven procurements. A key conclusion is the need for empowerment and flexibility within the context of best management practices for structuring procurements.

Technology Driven Procurements

Technology-driven procurements provide the ability to rapidly procure a new technology for evaluation or in the case where the procuring agency has designed a unique solution to meet the mission requirements of the users and is looking for a vendor to build the system to specification. This method is often a sole-source procurement as only one vendor has the right technology/capability at the time, leading to reduced cost for both the vendor and the procuring agency.

The DOE Office of Advanced Scientific Computing Research has supported a project called "Evaluation of Early System". The goals of the project are to select promising new technologies, acquire early versions of these technologies, rapidly deploy the new systems so that application scientists can get early access to the latest systems, and to publish the results of the evaluation. During the evaluation of the system, a suite of low level benchmarks, for example MPI ping-pong and the streams memory bandwidth test, kernel applications, for example, the Parallel Spectral Method Shallow Water Transport test and the NAS Parallel Benchmarks, and full applications are tested and compared to other available systems to understand the strengths and weaknesses of the various machines in terms of both hardware and software. This information is then made available to the public as openly as possible (subject to non-disclosure agreements) to aid others in the procurement process and to help in defining future directions for the procurement of high-end architectures

As HEC procurements shift from the vendor-proprietary (e.g., IBM SP with Power microprocessors and AIX) solution space to commodity hardware and Open Source software solutions, there are many more choices that can be made by the purchaser from Intel/AMD ecosystems for cluster components. That is, the purchaser can choose, among other things, the processor (e.g., IA-32, IA-64, IA32-64), node (e.g., dual or quad processors), interconnect (e.g., Quadrics, Infiniband or Myrinet), cluster management hardware and software, and packaging solutions. The procuring center would use a technology-driven procurement process to acquire a large commodity cluster built around a center-specific design based on a myriad of choices from the space of potential solutions. In so doing, the center can maximize performance/cost, but inherently assumes more risk and responsibility in the success of the HEC system.

A main advantage of this style of procurement is that it yields a system that is highly tuned to the technical requirements of the procuring center and can be accomplished quickly in a rapidly changing marketplace. By using this strategy, centers have been able to go from a technology announcement to having a world class computer running in as few as three months (although the average time varies). A second advantage is that the price can be very attractive because the vendors incur less pre-sales and proposal costs as well as much lower component and integration costs. Higher discounts have been obtained from commodity cluster procurements designed for the commodity market because of economies of scale and the volume distribution method increases competition and decreases margins at every level of the supply chain. Another advantage of this style of procurement is that it becomes feasible for centers to offset costs and increase the possibility of success by entering into close collaborations with vendors. By collaborating with the manufacturers, important information is passed to the system designers about the unique ways that scientific and technical applications stress the processors, memory, storage, and network subsystems of these machines. This technical exchange is beneficial to the center, the ultimate users in the scientific and engineering community, and the manufacturers, as it allows them to develop products better suited to HEC as well as to commercial customers.

Science Driven Procurements

Whereas the technology-driven procurement is tailored towards rapid evaluation of new systems or systems where the computer center has done substantial system design work, it is essential that major investments in computing technology be driven by scientific, programmatic, and/or mission requirements. Open, competitive procurements based on these requirements are one of the best ways to acquire a solution that meet the needs and requirements of the user community. Open procurements are often appropriate when there is the possibility of more than one effective solution, the scale of the system(s) is large, and/or it is mission-critical.

Regardless of the specific process chosen, open procurements start with assessing the scientific mission requirements, which involves forming a working team of scientific users, stakeholders, and the selection team. The requirements are translated into technical specifications that match the scientific mission requirements to the best technical options within the available budget. This matching is often reflected in tests or benchmarks that suppliers perform. Often there is interaction with the scientific user community, and possibly the suppliers, as the derived requirements and tests get refined. The principal task of the acquisition team is to decide the best alternative among the available choices based on current data. The effort involved both by the selection team and the suppliers depends less on the type of process chosen than on the sophistication of the testing. Due to the complexity of predicting behavior on future architectures it is important to have a balanced procurement team with expertise in computer hardware, operating systems and management, computer scientists who understand advanced architectures and algorithms, applied mathematicians who understand the implementation of algorithms, and user software developers who know the science to be done as well as the scaling of the algorithms.

Current Best Value Source Selection (BVSS) style procurements vary widely in implementation, are very flexible, and do not force the selection of the lowest bidder but result in

the solution with the best value. The results of such procurements range from cooperative research and development contracts to firm fixed price contracts.

Procurements should be focused on fulfilling the requirements of the user community and the stakeholder customers as opposed to prescribing implementation details and features that are more the purview of the vendor. Traditional system specification based procurements focus on the detailed design of a system by specifying many of the internal parameters of the potential system. The BVSS procurement process, currently used for most HEC systems, accomplishes this by describing a relatively small set of key requirements. This provides an opportunity for vendor innovation in addressing the requirements and recognizes that widely differing solutions cannot be encompassed in a detailed manner, but must be broader. Best Value methods provide more flexibility and are very cost effective. The evaluation of vendor responses is necessarily qualitative with the emphasis on the total solution as opposed to detailed feature-by-feature comparisons. The most common metric by which to compare disparate vendor responses is Time-To-Solution (TTS). TTS includes the development, pre- and post-processing times for an application. By having more than one supplier involved in a full or limited competitive procurement, the purchasing centers have the advantage of more information and options from which to choose. There is also the possibility that good solutions may come from sources that are not originally expected. The supplier competition often provides substantially lower costs and a more effective solution. Should the preferred option not perform as expected, this competition will already have identified an alternative solution.

Due to the scale of the largest system procurements being undertaken today, full-scale benchmarking for the performance requirements of targeted scientific applications is difficult if not impossible. Nevertheless, the sheer scale of the systems may introduce design considerations that will not surface using prototype benchmarking at smaller scale. Recent successes in performance benchmarking suggest an approach to a solution for this problem. For example, at Los Alamos, accurate performance models for applications from the ASCI workload have been developed and used for system design, optimization and maintenance, and have even been used in the procurement process for the ASCI Purple machine at LLNL, predicting the performance of the code SAGE on all the competing machines. These results suggest that it is possible to accurately predict the performance achieved by a future system (much larger in size and employing a distinct design from hardware currently in operation) running a future scientific application (much larger in problem size than currently being run), thereby allowing the decision makers to have at their disposal not only performance information but more importantly being able to analyze “what if” scenarios.

Expectations for success vary and must be clear

Whether implicit or explicit, with large-scale procurements there are a wide range of groups with expectations – the suppliers, the purchasers, the end users and the stakeholders who fund the systems. The end users can have widely different goals ranging from the design, evaluation, and testing of new architectures to the development of application software to the solution of complex domain-specific problems. It is essential that accurate and meaningful expectations be

set during the procurement process. Whereas procurement costs can be significant for both purchasers and the suppliers, they are relatively small compared to the resulting value and costs for the purchaser and supplier on large scale systems. No matter what method is used to enter a contract, much of the cost associated with the procurement is in defining the parameters of the contract. It is in the purchaser's as well as the supplier's best interest to have contracts that set clear expectations and parameters for success. If the solution is loosely- or under-specified, the technical solutions will not live up to the expectations of the purchasers and their clients. A poorly written contract can also become a problem for suppliers who then face large uncertain risk and to the purchasers who then have to continually renegotiate the terms of the contract. Even in the case of very fast procurements, there have been examples where the contract negotiations have taken significant additional time in order to set the proper expectations.

Thus it is important for all parties to fully understand and accept the requirements, the expected performance and the risks. The more uncertainty there is in the proposed solution, the more important it is to fully document the requirements and commitments. This effort requires resources and cost on both sides, but is essential.

Conclusion

Methods used to purchase existing standardized commodity systems simply do not scale to serve HEC procurements. There are some clear ways to improve and streamline the process. Laboratories have developed innovative methods that have been proven effective and should be allowed to continue these approaches. If all the Federal Acquisition Regulations applied directly to the Laboratories, the current BVSS and other processes discussed above would need to be completely redesigned or even totally abandoned.

How can the Federal Government improve the process? The goal is to be able to do performance driven procurements instead of ones that design the system *a priori*. Specific suggestions for improvements include: allowing for different solutions to unique situations including simultaneous negotiations with multiple vendors; enabling more open and iterative communications about true needs and requirements with the vendors; allowing multiple and flexible options for bigger/extra systems that can be exercised quickly; and allowing unscored and/or unweighted evaluations. Furthermore, it is clear that adjusting the traditional guidance for issues such as Intellectual Property, Indemnification, and Limitation of Liability would make the procurement process, or at least contract negotiations, faster and more effective. Potential vendors should be encouraged to get directly involved with the science mission themselves. Once the science mission collaboration is established it will produce a team where the vendor/center has a system defined to better meet the scientific needs. In order to improve the state of High End Computing, it is critical that the methods used to acquire the systems and services be revitalized as well. There needs to be room for flexibility, creativity and cooperation within the procurement process, while still assuring the systems obtained meet the science mission driven requirements.